



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:09 PM UTC

PDB ID : 7K5H / pdb_00007k5h
Title : 1.90 Å resolution structure of WT BfrB from *Pseudomonas aeruginosa* in complex with a protein-protein interaction inhibitor KM-5-66
Authors : Lovell, S.; Battaile, K.P.; Soldano, A.; Punchi-Hewage, A.; Meraz, K.; Annor-Gyamfi, J.K.; Yao, H.; Bunce, R.A.; Rivera, M.
Deposited on : 2020-09-16
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

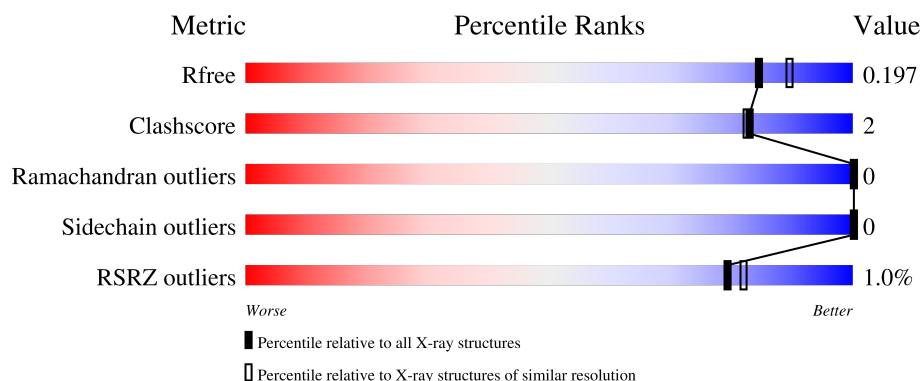
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	158	0% 97% ..
1	B	158	0% 92% 6% .
1	C	158	2% 94% ..
1	D	158	0% 93% 6% .

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Mol	Chain	Length	Quality of chain
1	E	158	% 92% 6% .
1	F	158	% 93% 6% .
1	G	158	% 95% . .
1	H	158	% 96% . .
1	I	158	% 94% . .
1	J	158	% 92% 6% .
1	K	158	% 93% 6% .
1	L	158	2% 96% . .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 16725 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ferroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	S	0	1	0
			1272	807	218	240	7			
1	B	156	Total	C	N	O	S	0	1	0
			1266	802	216	241	7			
1	C	156	Total	C	N	O	S	0	1	0
			1267	801	216	243	7			
1	D	156	Total	C	N	O	S	0	1	0
			1263	799	216	241	7			
1	E	156	Total	C	N	O	S	0	2	0
			1272	806	216	243	7			
1	F	156	Total	C	N	O	S	0	1	0
			1261	800	215	239	7			
1	G	156	Total	C	N	O	S	0	1	0
			1266	802	215	242	7			
1	H	156	Total	C	N	O	S	0	2	0
			1275	807	217	244	7			
1	I	156	Total	C	N	O	S	0	1	0
			1269	803	215	244	7			
1	J	156	Total	C	N	O	S	0	1	0
			1268	802	216	243	7			
1	K	156	Total	C	N	O	S	0	1	0
			1264	801	214	242	7			
1	L	156	Total	C	N	O	S	0	2	0
			1270	806	216	241	7			

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

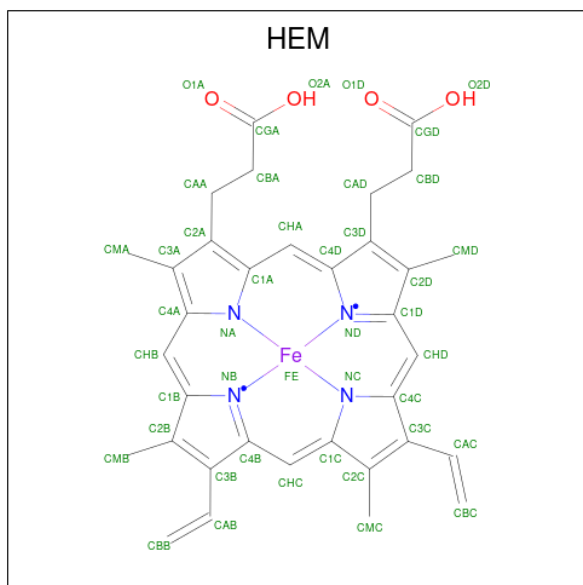
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	K	0	0
			1	1		
2	B	1	Total	K	0	0
			1	1		

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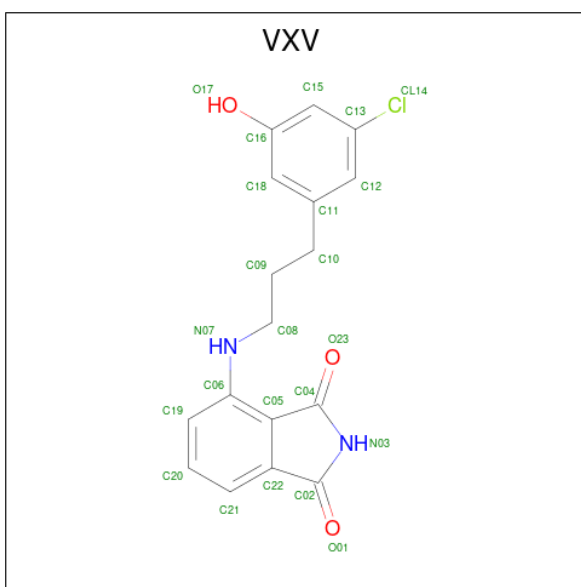
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total K 1 1	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C Fe N O 43 34 1 4 4	0	0
3	C	1	Total C Fe N O 43 34 1 4 4	0	0
3	D	1	Total C Fe N O 43 34 1 4 4	0	0
3	E	1	Total C Fe N O 43 34 1 4 4	0	0
3	F	1	Total C Fe N O 43 34 1 4 4	0	0
3	H	1	Total C Fe N O 43 34 1 4 4	0	0
3	L	1	Total C Fe N O 43 34 1 4 4	0	0

- Molecule 4 is 4-{{3-(3-chloro-5-hydroxyphenyl)propyl}amino}-1H-isoindole-1,3(2H)-dione (CCD ID: VXV) (formula: $C_{17}H_{15}ClN_2O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 13 9 2 2	0	0
4	B	1	Total C Cl N O 23 17 1 2 3	0	0
4	C	1	Total C N O 15 11 2 2	0	0
4	C	1	Total C Cl N O 23 17 1 2 3	0	0
4	D	1	Total C N O 12 8 2 2	0	0
4	E	1	Total C N O 16 12 2 2	0	0
4	F	1	Total C Cl N O 23 17 1 2 3	0	0
4	H	1	Total C N O 15 11 2 2	0	0
4	J	1	Total C N O 16 12 2 2	0	0
4	K	1	Total C Cl N O 23 17 1 2 3	0	0
4	L	1	Total C N O 14 10 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	88	Total O 88 88	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	86	Total 86	O 86	0	0
5	C	85	Total 85	O 85	0	0
5	D	75	Total 75	O 75	0	0
5	E	83	Total 83	O 83	0	0
5	F	79	Total 79	O 79	0	0
5	G	80	Total 80	O 80	0	0
5	H	84	Total 84	O 84	0	0
5	I	79	Total 79	O 79	0	0
5	J	92	Total 92	O 92	0	0
5	K	99	Total 99	O 99	0	0
5	L	85	Total 85	O 85	0	0

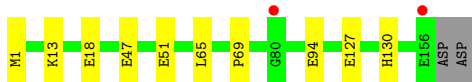
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Ferroxidase



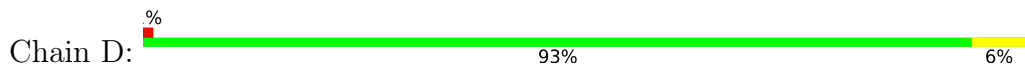
- Molecule 1: Ferroxidase



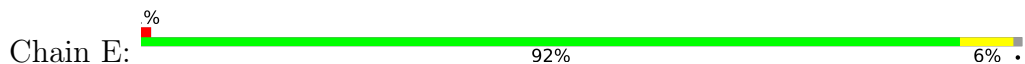
- Molecule 1: Ferroxidase



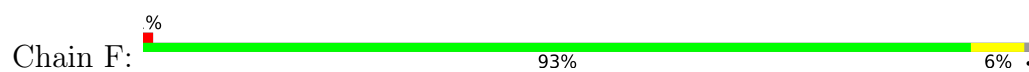
- Molecule 1: Ferroxidase



- Molecule 1: Ferroxidase



- Molecule 1: Ferroxidase



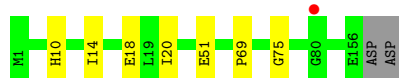
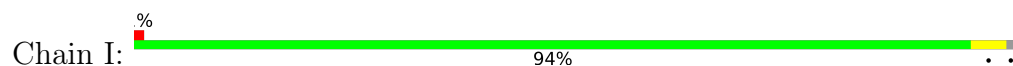
● Molecule 1: Ferroxidase



● Molecule 1: Ferroxidase



● Molecule 1: Ferroxidase



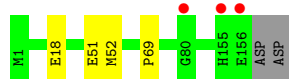
● Molecule 1: Ferroxidase



● Molecule 1: Ferroxidase



● Molecule 1: Ferroxidase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	129.50Å 194.50Å 202.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.78 – 1.90 46.78 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.78-1.90) 100.0 (46.78-1.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 1.90Å)	Xtriage
Refinement program	PHENIX dev_3959	Depositor
R, R_{free}	0.158 , 0.189 0.168 , 0.197	Depositor DCC
R_{free} test set	10033 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	25.9	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16725	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: K, HEM, VXV

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.40	0/1296	0.53	0/1745
1	B	0.39	0/1290	0.48	0/1740
1	C	0.42	0/1291	0.52	0/1742
1	D	0.35	0/1287	0.50	0/1737
1	E	0.42	0/1299	0.51	0/1752
1	F	0.40	0/1285	0.49	0/1734
1	G	0.38	0/1290	0.49	0/1740
1	H	0.40	0/1302	0.50	0/1756
1	I	0.39	0/1293	0.51	0/1744
1	J	0.42	0/1292	0.52	0/1743
1	K	0.37	0/1288	0.52	0/1738
1	L	0.39	0/1297	0.48	0/1749
All	All	0.40	0/15510	0.50	0/20920

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1272	0	1254	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1266	0	1231	7	0
1	C	1267	0	1229	5	0
1	D	1263	0	1225	6	0
1	E	1272	0	1237	7	0
1	F	1261	0	1222	6	0
1	G	1266	0	1229	3	0
1	H	1275	0	1241	4	0
1	I	1269	0	1231	4	0
1	J	1268	0	1231	6	0
1	K	1264	0	1222	6	0
1	L	1270	0	1237	3	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	D	1	0	0	0	0
3	A	43	0	30	2	0
3	C	43	0	30	4	0
3	D	43	0	30	0	0
3	E	43	0	30	5	0
3	F	43	0	30	4	0
3	H	43	0	30	6	0
3	L	43	0	30	1	0
4	A	13	0	0	1	0
4	B	23	0	0	2	0
4	C	38	0	0	2	0
4	D	12	0	0	1	0
4	E	16	0	0	0	0
4	F	23	0	0	1	0
4	H	15	0	0	1	0
4	J	16	0	0	1	0
4	K	23	0	0	1	0
4	L	14	0	0	1	0
5	A	88	0	0	0	0
5	B	86	0	0	1	0
5	C	85	0	0	0	0
5	D	75	0	0	0	0
5	E	83	0	0	1	0
5	F	79	0	0	0	0
5	G	80	0	0	0	0
5	H	84	0	0	0	0
5	I	79	0	0	0	0
5	J	92	0	0	0	0
5	K	99	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	85	0	0	0	0
All	All	16725	0	14999	74	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (74) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:201:HEM:HMC1	3:F:201:HEM:HBC2	1.49	0.95
3:E:201:HEM:HMC1	3:E:201:HEM:HBC2	1.67	0.76
3:A:202:HEM:HMC1	3:A:202:HEM:HBC2	1.73	0.71
3:F:201:HEM:HBC2	3:F:201:HEM:CMC	2.20	0.70
1:E:147[A]:GLU:H	1:E:147[A]:GLU:CD	2.06	0.63
1:J:82:ASN:OD1	1:J:84:GLN:HG2	1.99	0.63
3:E:201:HEM:HBC2	3:E:201:HEM:CMC	2.29	0.62
3:H:201:HEM:HMC2	3:H:201:HEM:HBC2	1.82	0.60
1:K:18:GLU:OE1	1:K:51:GLU:OE1	2.20	0.60
1:F:18:GLU:OE1	1:F:51:GLU:OE1	2.21	0.59
1:C:18:GLU:OE1	1:C:51:GLU:OE1	2.20	0.59
3:H:201:HEM:HBC2	3:H:201:HEM:CMC	2.33	0.59
1:D:18:GLU:OE1	1:D:51:GLU:OE1	2.21	0.58
1:E:18:GLU:OE1	1:E:51:GLU:OE1	2.22	0.58
3:A:202:HEM:HBC2	3:A:202:HEM:CMC	2.33	0.58
1:I:18:GLU:OE1	1:I:51:GLU:OE1	2.21	0.58
1:B:18:GLU:OE1	1:B:51:GLU:OE1	2.22	0.57
3:C:201:HEM:HMC2	3:C:201:HEM:HBC2	1.89	0.55
3:C:201:HEM:HBC2	3:C:201:HEM:CMC	2.37	0.55
1:H:18:GLU:OE1	1:H:51:GLU:OE1	2.26	0.54
1:J:18:GLU:OE1	1:J:51:GLU:OE1	2.26	0.53
3:E:201:HEM:CMB	3:E:201:HEM:HBB2	2.38	0.53
1:C:47:GLU:OE1	1:C:130:HIS:CD2	2.62	0.53
3:H:201:HEM:CMB	3:H:201:HEM:HBB2	2.39	0.52
3:C:201:HEM:CMB	3:C:201:HEM:HBB2	2.40	0.52
1:G:18:GLU:OE1	1:G:51:GLU:OE1	2.27	0.52
1:J:69:PRO:O	4:J:201:VXV:N03	2.44	0.50
1:L:69:PRO:O	4:L:202:VXV:N03	2.45	0.50
1:K:20:ILE:HG23	1:K:77:LEU:HD12	1.93	0.50
1:I:10:HIS:O	1:I:14:ILE:HG12	2.12	0.50
1:D:47:GLU:OE1	1:D:130:HIS:NE2	2.45	0.50
1:L:52:MET:HB3	3:L:201:HEM:CHD	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:134:LEU:HD21	5:E:311:HOH:O	2.13	0.49
1:K:69:PRO:O	4:K:201:VXV:N03	2.46	0.49
4:C:203:VXV:N03	1:I:69:PRO:O	2.46	0.48
1:I:20:ILE:HD11	1:I:75:GLY:HA3	1.96	0.48
1:H:52:MET:HB3	3:H:201:HEM:CHD	2.44	0.48
1:F:69:PRO:O	4:F:202:VXV:N03	2.47	0.47
1:L:18:GLU:OE1	1:L:51:GLU:OE1	2.32	0.47
1:C:69:PRO:O	4:C:202:VXV:N03	2.48	0.47
1:C:47:GLU:OE1	1:C:130:HIS:NE2	2.48	0.47
1:B:47:GLU:OE1	1:B:130:HIS:CD2	2.68	0.47
1:G:44:GLU:OE2	1:G:90:ASP:OD2	2.33	0.47
1:C:20:ILE:HD11	1:C:75:GLY:HA3	1.98	0.46
1:A:20:ILE:HD11	1:A:75:GLY:HA3	1.98	0.46
1:F:52:MET:HB3	3:F:201:HEM:CHD	2.46	0.45
1:B:47:GLU:OE1	1:B:130:HIS:NE2	2.50	0.45
1:D:69:PRO:O	4:D:203:VXV:N03	2.50	0.45
1:E:52:MET:HB3	3:E:201:HEM:CHB	2.47	0.45
1:A:69:PRO:O	4:A:203:VXV:N03	2.50	0.44
1:K:1:MET:O	1:K:65:LEU:HA	2.18	0.44
1:B:69:PRO:O	4:B:202:VXV:N03	2.51	0.43
1:F:44:GLU:OE2	1:F:90:ASP:OD2	2.36	0.43
1:H:69:PRO:O	4:H:202:VXV:N03	2.51	0.43
4:B:202:VXV:C18	1:E:81:GLU:HA	2.49	0.43
3:E:201:HEM:HBB2	3:E:201:HEM:HMB1	1.99	0.43
1:D:10:HIS:O	1:D:14:ILE:HG12	2.19	0.42
3:F:201:HEM:CHB	1:K:52:MET:HB3	2.49	0.42
1:B:1:MET:O	1:B:65:LEU:HA	2.20	0.42
1:E:44:GLU:OE2	1:E:90:ASP:OD2	2.36	0.42
1:H:52:MET:HB3	3:H:201:HEM:C1D	2.54	0.42
1:F:51:GLU:OE2	1:F:130:HIS:HE1	2.03	0.42
1:D:47:GLU:OE1	1:D:130:HIS:CD2	2.73	0.42
1:B:13:LYS:NZ	5:B:309:HOH:O	2.53	0.41
1:J:20:ILE:HG23	1:J:77:LEU:HD12	2.01	0.41
1:K:20:ILE:HD11	1:K:75:GLY:HA3	2.03	0.41
1:B:94:GLU:OE1	1:B:127:GLU:OE1	2.38	0.41
1:J:44:GLU:OE2	1:J:90:ASP:OD2	2.39	0.41
1:E:10:HIS:O	1:E:14:ILE:HG12	2.20	0.41
3:C:201:HEM:HBB2	3:C:201:HEM:HMB1	2.02	0.41
1:D:20:ILE:HD11	1:D:75:GLY:HA3	2.03	0.41
1:F:28:HIS:NE2	1:F:79:ILE:O	2.42	0.41
1:G:1:MET:O	1:G:65:LEU:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:201:HEM:CHB	1:J:52:MET:HB3	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	155/158 (98%)	154 (99%)	1 (1%)	0	100	100
1	B	155/158 (98%)	154 (99%)	1 (1%)	0	100	100
1	C	155/158 (98%)	154 (99%)	1 (1%)	0	100	100
1	D	155/158 (98%)	154 (99%)	1 (1%)	0	100	100
1	E	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
1	F	155/158 (98%)	154 (99%)	1 (1%)	0	100	100
1	G	155/158 (98%)	153 (99%)	2 (1%)	0	100	100
1	H	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
1	I	155/158 (98%)	154 (99%)	1 (1%)	0	100	100
1	J	155/158 (98%)	153 (99%)	2 (1%)	0	100	100
1	K	155/158 (98%)	155 (100%)	0	0	100	100
1	L	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
All	All	1863/1896 (98%)	1850 (99%)	13 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar

resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	137/144 (95%)	137 (100%)	0	100	100
1	B	135/144 (94%)	135 (100%)	0	100	100
1	C	136/144 (94%)	136 (100%)	0	100	100
1	D	135/144 (94%)	135 (100%)	0	100	100
1	E	136/144 (94%)	136 (100%)	0	100	100
1	F	133/144 (92%)	133 (100%)	0	100	100
1	G	135/144 (94%)	135 (100%)	0	100	100
1	H	137/144 (95%)	137 (100%)	0	100	100
1	I	136/144 (94%)	136 (100%)	0	100	100
1	J	136/144 (94%)	136 (100%)	0	100	100
1	K	134/144 (93%)	134 (100%)	0	100	100
1	L	135/144 (94%)	135 (100%)	0	100	100
All	All	1625/1728 (94%)	1625 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	HIS
1	A	137	GLN
1	B	43	HIS
1	B	46	HIS
1	B	88	GLN
1	C	84	GLN
1	C	88	GLN
1	D	88	GLN
1	D	155	HIS
1	E	88	GLN
1	F	130	HIS
1	H	43	HIS
1	I	43	HIS
1	J	112	HIS
1	K	84	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 3 are monoatomic - leaving 18 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	VXV	D	203	-	13,13,25	1.40	3 (23%)	17,19,35	2.85	6 (35%)
3	HEM	E	201	1	50,50,50	1.43	7 (14%)	67,82,82	1.25	9 (13%)
4	VXV	B	202	-	25,25,25	1.69	6 (24%)	35,35,35	2.56	14 (40%)
4	VXV	F	202	-	25,25,25	1.56	6 (24%)	35,35,35	2.24	10 (28%)
4	VXV	H	202	-	16,16,25	1.91	4 (25%)	22,22,35	2.07	8 (36%)
3	HEM	D	202	1	50,50,50	1.39	9 (18%)	67,82,82	1.20	6 (8%)
4	VXV	J	201	-	17,17,25	1.62	3 (17%)	23,23,35	2.55	8 (34%)
4	VXV	K	201	-	25,25,25	1.62	5 (20%)	35,35,35	2.22	11 (31%)
3	HEM	A	202	1	50,50,50	1.42	10 (20%)	67,82,82	1.33	8 (11%)
3	HEM	L	201	1	50,50,50	1.45	7 (14%)	67,82,82	1.24	4 (5%)
4	VXV	A	203	-	14,14,25	1.93	4 (28%)	19,20,35	3.03	9 (47%)
3	HEM	F	201	1	50,50,50	1.44	9 (18%)	67,82,82	1.26	8 (11%)
4	VXV	C	202	-	16,16,25	1.81	5 (31%)	22,22,35	2.46	8 (36%)
4	VXV	E	202	-	17,17,25	1.67	5 (29%)	23,23,35	2.50	9 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	VXV	C	203	-	25,25,25	1.90	7 (28%)	35,35,35	2.19	10 (28%)
4	VXV	L	202	-	15,15,25	1.46	3 (20%)	21,21,35	2.56	10 (47%)
3	HEM	C	201	1	50,50,50	1.50	10 (20%)	67,82,82	1.29	9 (13%)
3	HEM	H	201	1	50,50,50	1.50	8 (16%)	67,82,82	1.45	10 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	VXV	D	203	-	-	-	0/2/2/3
3	HEM	E	201	1	-	4/14/54/54	-
4	VXV	B	202	-	-	0/7/19/19	0/3/3/3
4	VXV	F	202	-	-	1/7/19/19	0/3/3/3
4	VXV	H	202	-	-	0/4/16/19	0/2/2/3
3	HEM	D	202	1	-	4/14/54/54	-
4	VXV	J	201	-	-	0/5/17/19	0/2/2/3
4	VXV	K	201	-	-	1/7/19/19	0/3/3/3
3	HEM	A	202	1	-	4/14/54/54	-
3	HEM	L	201	1	-	4/14/54/54	-
4	VXV	A	203	-	-	0/2/14/19	0/2/2/3
3	HEM	F	201	1	-	4/14/54/54	-
4	VXV	C	202	-	-	0/4/16/19	0/2/2/3
4	VXV	E	202	-	-	0/5/17/19	0/2/2/3
4	VXV	C	203	-	-	2/7/19/19	0/3/3/3
4	VXV	L	202	-	-	0/3/15/19	0/2/2/3
3	HEM	C	201	1	-	2/14/54/54	-
3	HEM	H	201	1	-	4/14/54/54	-

All (111) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	203	VXV	C06-N07	4.95	1.46	1.37
3	C	201	HEM	FE-ND	4.43	2.08	1.94
3	L	201	HEM	FE-ND	4.35	2.08	1.94
3	F	201	HEM	FE-NA	4.34	2.09	1.95
3	A	202	HEM	FE-ND	4.27	2.08	1.94
4	H	202	VXV	C02-N03	-4.22	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	201	HEM	FE-ND	4.12	2.07	1.94
4	J	201	VXV	C06-N07	4.08	1.48	1.37
3	H	201	HEM	FE-NA	4.06	2.08	1.95
4	B	202	VXV	C06-N07	4.04	1.48	1.37
4	C	203	VXV	C13-CL14	4.03	1.83	1.74
3	E	201	HEM	FE-NA	3.98	2.08	1.95
4	K	201	VXV	C15-C16	-3.97	1.33	1.39
3	D	202	HEM	FE-ND	3.92	2.07	1.94
4	H	202	VXV	C06-N07	3.88	1.47	1.37
4	C	202	VXV	C06-N07	3.77	1.47	1.37
4	E	202	VXV	C06-N07	3.76	1.47	1.37
4	B	202	VXV	C02-N03	-3.63	1.33	1.38
3	H	201	HEM	FE-NB	3.59	2.06	1.94
3	L	201	HEM	FE-NA	3.56	2.06	1.95
3	H	201	HEM	FE-ND	3.50	2.05	1.94
4	F	202	VXV	C06-N07	3.49	1.46	1.37
3	A	202	HEM	FE-NA	3.41	2.06	1.95
4	C	203	VXV	C06-N07	3.33	1.46	1.37
4	F	202	VXV	C20-C21	3.31	1.44	1.38
4	E	202	VXV	C20-C21	3.26	1.44	1.38
3	D	202	HEM	FE-NA	3.20	2.05	1.95
4	A	203	VXV	C02-N03	-3.18	1.33	1.38
3	C	201	HEM	FE-NA	3.18	2.05	1.95
4	K	201	VXV	C06-N07	3.10	1.45	1.37
4	L	202	VXV	C06-N07	3.02	1.45	1.37
3	F	201	HEM	FE-ND	3.01	2.04	1.94
4	F	202	VXV	C20-C19	2.97	1.44	1.38
4	B	202	VXV	C20-C21	2.96	1.44	1.38
3	A	202	HEM	FE-NC	2.96	2.04	1.95
3	L	201	HEM	CAB-C3B	2.94	1.55	1.47
4	C	203	VXV	C20-C21	2.93	1.43	1.38
4	L	202	VXV	C20-C21	2.91	1.43	1.38
3	C	201	HEM	FE-NB	2.91	2.03	1.94
3	F	201	HEM	FE-NB	2.89	2.03	1.94
4	C	202	VXV	C02-N03	-2.85	1.34	1.38
4	C	203	VXV	O17-C16	2.83	1.43	1.37
3	D	202	HEM	CAB-C3B	2.82	1.54	1.47
4	D	203	VXV	C06-N07	2.81	1.47	1.38
4	D	203	VXV	C02-N03	-2.80	1.34	1.38
3	L	201	HEM	FE-NB	2.79	2.03	1.94
4	C	202	VXV	C20-C21	2.78	1.43	1.38
3	L	201	HEM	CAC-C3C	2.77	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	201	VXV	C20-C21	2.76	1.43	1.38
4	C	203	VXV	C02-N03	-2.76	1.34	1.38
3	H	201	HEM	FE-NC	2.74	2.04	1.95
3	H	201	HEM	CAC-C3C	2.67	1.54	1.47
3	L	201	HEM	FE-NC	2.67	2.04	1.95
4	C	203	VXV	C12-C13	2.67	1.42	1.38
3	D	202	HEM	CAC-C3C	2.67	1.54	1.47
3	C	201	HEM	CAC-C3C	2.66	1.54	1.47
3	A	202	HEM	CAB-C3B	2.60	1.54	1.47
3	A	202	HEM	CAC-C3C	2.59	1.54	1.47
3	C	201	HEM	CMC-C2C	2.58	1.56	1.50
3	F	201	HEM	CAC-C3C	2.58	1.54	1.47
3	C	201	HEM	CAB-C3B	2.55	1.54	1.47
3	E	201	HEM	CAC-C3C	2.55	1.54	1.47
3	D	202	HEM	FE-NB	2.55	2.02	1.94
3	C	201	HEM	CMD-C2D	2.54	1.56	1.50
3	E	201	HEM	CMB-C2B	2.51	1.55	1.50
3	F	201	HEM	CMC-C2C	2.50	1.55	1.50
3	F	201	HEM	FE-NC	2.49	2.03	1.95
4	C	202	VXV	C20-C19	2.48	1.43	1.38
3	E	201	HEM	CAB-C3B	2.48	1.54	1.47
3	D	202	HEM	FE-NC	2.46	2.03	1.95
3	A	202	HEM	CMC-C2C	2.45	1.55	1.50
3	F	201	HEM	CAB-C3B	2.44	1.53	1.47
3	H	201	HEM	CAB-C3B	2.43	1.53	1.47
4	A	203	VXV	C20-C19	2.42	1.43	1.38
3	E	201	HEM	CMC-C2C	2.42	1.55	1.50
4	H	202	VXV	C20-C21	2.40	1.43	1.38
4	K	201	VXV	C02-N03	-2.40	1.34	1.38
4	C	202	VXV	C22-C02	2.39	1.52	1.48
3	H	201	HEM	CMD-C2D	2.37	1.55	1.50
4	J	201	VXV	C20-C21	2.36	1.42	1.38
3	C	201	HEM	CMB-C2B	2.35	1.55	1.50
4	B	202	VXV	C20-C19	2.34	1.42	1.38
3	H	201	HEM	CMA-C3A	2.34	1.55	1.50
4	E	202	VXV	C20-C19	2.32	1.42	1.38
3	C	201	HEM	CMA-C3A	2.30	1.55	1.50
3	F	201	HEM	CMB-C2B	2.30	1.55	1.50
4	F	202	VXV	C15-C16	-2.29	1.35	1.39
4	F	202	VXV	O17-C16	2.29	1.42	1.37
3	C	201	HEM	FE-NC	2.28	2.02	1.95
4	C	203	VXV	C15-C13	2.27	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	202	HEM	CMA-C3A	2.27	1.55	1.50
4	F	202	VXV	C02-N03	-2.26	1.35	1.38
4	D	203	VXV	C20-C21	2.25	1.42	1.38
4	B	202	VXV	O17-C16	2.20	1.41	1.37
3	D	202	HEM	CMD-C2D	2.19	1.55	1.50
3	E	201	HEM	CMD-C2D	2.15	1.55	1.50
3	A	202	HEM	FE-NB	2.15	2.01	1.94
3	D	202	HEM	CMA-C3A	2.15	1.55	1.50
4	J	201	VXV	C09-C08	2.15	1.60	1.51
4	A	203	VXV	C20-C21	2.14	1.42	1.38
3	A	202	HEM	CMD-C2D	2.14	1.55	1.50
3	D	202	HEM	CMC-C2C	2.14	1.55	1.50
3	L	201	HEM	CMC-C2C	2.13	1.55	1.50
4	B	202	VXV	C15-C16	-2.09	1.36	1.39
4	E	202	VXV	C02-N03	-2.09	1.35	1.38
4	E	202	VXV	C22-C02	2.08	1.51	1.48
3	F	201	HEM	CMD-C2D	2.05	1.55	1.50
4	K	201	VXV	O17-C16	2.02	1.41	1.37
4	L	202	VXV	C20-C19	2.02	1.42	1.38
3	A	202	HEM	CMB-C2B	2.01	1.54	1.50
4	H	202	VXV	C05-C06	-2.00	1.37	1.41

All (157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	203	VXV	C04-N03-C02	-6.96	106.54	112.59
4	A	203	VXV	C04-N03-C02	-6.91	106.59	112.59
4	E	202	VXV	C04-N03-C02	-6.54	106.91	112.59
4	J	201	VXV	C04-N03-C02	-6.53	106.92	112.59
4	K	201	VXV	C04-N03-C02	-6.46	106.98	112.59
4	D	203	VXV	C22-C02-N03	6.28	111.29	105.88
4	A	203	VXV	C22-C02-N03	6.27	111.28	105.88
4	J	201	VXV	C22-C02-N03	6.08	111.12	105.88
4	L	202	VXV	C04-N03-C02	-6.06	107.32	112.59
4	F	202	VXV	C04-N03-C02	-6.00	107.37	112.59
4	C	203	VXV	C04-N03-C02	-5.99	107.39	112.59
4	B	202	VXV	C04-N03-C02	-5.84	107.52	112.59
4	B	202	VXV	C22-C02-N03	5.80	110.88	105.88
4	C	202	VXV	C04-N03-C02	-5.69	107.65	112.59
4	F	202	VXV	C22-C02-N03	5.30	110.44	105.88
4	K	201	VXV	C22-C02-N03	5.16	110.33	105.88
4	A	203	VXV	C06-C05-C04	5.04	134.93	129.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	203	VXV	C22-C02-N03	4.89	110.09	105.88
4	C	202	VXV	C22-C02-N03	4.88	110.09	105.88
4	A	203	VXV	C22-C05-C04	-4.85	103.67	108.09
4	L	202	VXV	C06-C05-C04	4.80	134.67	129.42
4	B	202	VXV	C06-C05-C04	4.71	134.57	129.42
4	E	202	VXV	C22-C02-N03	4.61	109.86	105.88
4	J	201	VXV	C06-C05-C04	4.60	134.45	129.42
4	D	203	VXV	C22-C05-C04	-4.57	103.92	108.09
4	C	203	VXV	C06-C05-C04	4.55	134.40	129.42
4	B	202	VXV	C22-C05-C04	-4.54	103.94	108.09
4	L	202	VXV	C22-C02-N03	4.53	109.78	105.88
4	C	203	VXV	C22-C05-C04	-4.36	104.11	108.09
4	K	201	VXV	C06-C05-C04	4.20	134.01	129.42
4	H	202	VXV	C22-C02-N03	4.17	109.47	105.88
4	E	202	VXV	C22-C05-C04	-4.09	104.36	108.09
4	F	202	VXV	C06-C05-C04	3.99	133.79	129.42
4	C	202	VXV	C22-C05-C04	-3.96	104.48	108.09
4	H	202	VXV	C06-C05-C04	3.93	133.72	129.42
4	J	201	VXV	C22-C05-C04	-3.90	104.53	108.09
4	K	201	VXV	C22-C05-C04	-3.90	104.53	108.09
4	L	202	VXV	C22-C05-C04	-3.80	104.63	108.09
4	C	202	VXV	C06-C05-C04	3.78	133.56	129.42
4	E	202	VXV	C06-C05-C04	3.78	133.55	129.42
4	B	202	VXV	C12-C13-CL14	-3.59	114.66	119.17
4	F	202	VXV	C22-C05-C04	-3.59	104.81	108.09
4	H	202	VXV	C22-C05-C04	-3.56	104.84	108.09
4	F	202	VXV	C05-C22-C02	-3.55	105.02	108.18
4	B	202	VXV	C05-C22-C02	-3.53	105.04	108.18
4	C	202	VXV	C05-C22-C02	-3.46	105.10	108.18
4	F	202	VXV	C18-C16-C15	3.42	125.16	120.47
4	B	202	VXV	C16-C15-C13	-3.37	113.87	118.67
3	H	201	HEM	C1B-NB-C4B	3.33	109.14	105.21
4	B	202	VXV	C18-C16-C15	3.32	125.03	120.47
4	K	201	VXV	C18-C16-C15	3.28	124.98	120.47
3	H	201	HEM	C4D-ND-C1D	3.28	109.09	105.21
3	F	201	HEM	CHC-C4B-NB	3.25	127.92	124.42
4	H	202	VXV	C05-C22-C02	-3.22	105.31	108.18
4	F	202	VXV	C16-C15-C13	-3.19	114.12	118.67
4	E	202	VXV	C21-C22-C02	3.17	135.46	129.32
4	B	202	VXV	C10-C11-C18	3.15	125.83	120.54
4	B	202	VXV	C21-C22-C02	3.13	135.37	129.32
4	C	202	VXV	C21-C22-C02	3.07	135.26	129.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	203	VXV	C21-C22-C02	3.03	135.17	129.32
4	C	203	VXV	C05-C22-C02	-2.89	105.61	108.18
3	H	201	HEM	C3D-C4D-ND	-2.85	107.05	110.17
3	H	201	HEM	CHC-C4B-NB	2.83	127.47	124.42
4	H	202	VXV	C21-C22-C02	2.81	134.77	129.32
4	L	202	VXV	C05-C22-C02	-2.80	105.68	108.18
3	H	201	HEM	C3B-C4B-NB	-2.80	107.46	109.47
3	A	202	HEM	C4D-ND-C1D	2.79	108.51	105.21
3	E	201	HEM	C4D-ND-C1D	2.78	108.50	105.21
3	C	201	HEM	C1B-NB-C4B	2.77	108.49	105.21
3	A	202	HEM	C1B-NB-C4B	2.74	108.46	105.21
4	C	203	VXV	C18-C16-C15	2.74	124.23	120.47
3	D	202	HEM	C4D-ND-C1D	2.74	108.45	105.21
4	B	202	VXV	O01-C02-N03	-2.73	117.78	125.60
3	H	201	HEM	C2B-C1B-NB	-2.73	106.70	109.84
3	L	201	HEM	C1B-NB-C4B	2.72	108.42	105.21
4	K	201	VXV	C21-C22-C02	2.70	134.55	129.32
3	E	201	HEM	CBA-CAA-C2A	-2.69	105.10	112.53
4	F	202	VXV	C21-C22-C02	2.65	134.46	129.32
4	L	202	VXV	C21-C22-C02	2.65	134.45	129.32
4	D	203	VXV	C05-C22-C02	-2.61	105.85	108.18
4	E	202	VXV	C05-C22-C02	-2.60	105.87	108.18
3	C	201	HEM	C4D-ND-C1D	2.59	108.28	105.21
4	C	202	VXV	O01-C02-N03	-2.59	118.20	125.60
3	F	201	HEM	C2A-C1A-NA	-2.59	107.28	110.15
4	F	202	VXV	C08-N07-C06	2.55	129.54	123.35
3	H	201	HEM	CAD-CBD-CGD	-2.55	106.90	113.67
4	A	203	VXV	O01-C02-N03	-2.55	118.32	125.60
3	H	201	HEM	C3B-C2B-C1B	2.54	108.32	106.41
3	L	201	HEM	C3B-C2B-C1B	2.54	108.32	106.41
4	H	202	VXV	C04-N03-C02	-2.54	110.38	112.59
3	C	201	HEM	C3B-C4B-NB	-2.53	107.65	109.47
4	E	202	VXV	C08-N07-C06	2.52	129.46	123.35
4	C	203	VXV	O01-C02-N03	-2.52	118.40	125.60
4	K	201	VXV	C16-C15-C13	-2.49	115.12	118.67
3	E	201	HEM	C4C-C3C-C2C	2.49	108.97	106.81
4	H	202	VXV	O01-C02-N03	-2.48	118.50	125.60
4	J	201	VXV	C05-C22-C02	-2.48	105.97	108.18
4	E	202	VXV	O01-C02-N03	-2.47	118.54	125.60
3	L	201	HEM	C4D-ND-C1D	2.46	108.12	105.21
4	A	203	VXV	C05-C22-C02	-2.43	106.02	108.18
4	B	202	VXV	C10-C11-C12	-2.42	116.47	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	202	HEM	C2A-C1A-NA	-2.42	107.47	110.15
3	E	201	HEM	C1B-NB-C4B	2.41	108.06	105.21
3	A	202	HEM	C3D-C4D-ND	-2.39	107.55	110.17
3	E	201	HEM	CHC-C4B-NB	2.38	126.99	124.42
4	D	203	VXV	C21-C22-C02	2.37	133.92	129.32
3	D	202	HEM	C3D-C4D-ND	-2.36	107.58	110.17
3	D	202	HEM	C2A-C1A-NA	-2.35	107.54	110.15
3	A	202	HEM	CHC-C4B-NB	2.35	126.95	124.42
3	C	201	HEM	CHC-C1C-NC	2.35	127.01	124.45
4	F	202	VXV	O01-C02-N03	-2.35	118.90	125.60
3	C	201	HEM	C2A-C1A-NA	-2.33	107.57	110.15
3	H	201	HEM	C2A-C1A-NA	-2.33	107.57	110.15
4	A	203	VXV	C08-N07-C06	2.32	126.04	122.37
3	F	201	HEM	C4D-ND-C1D	2.32	107.95	105.21
4	B	202	VXV	C16-C18-C11	-2.31	118.67	120.35
4	A	203	VXV	C21-C22-C02	2.31	133.79	129.32
3	F	201	HEM	C1B-NB-C4B	2.29	107.92	105.21
4	L	202	VXV	C22-C05-C06	-2.28	120.70	121.88
3	F	201	HEM	C3B-C4B-NB	-2.27	107.84	109.47
4	J	201	VXV	O01-C02-N03	-2.26	119.14	125.60
3	D	202	HEM	C1B-NB-C4B	2.24	107.86	105.21
3	F	201	HEM	C4C-C3C-C2C	2.23	108.75	106.81
3	C	201	HEM	CAD-CBD-CGD	-2.23	107.74	113.67
4	K	201	VXV	O01-C02-N03	-2.23	119.22	125.60
4	L	202	VXV	C08-N07-C06	2.23	127.89	123.22
3	H	201	HEM	CHA-C4D-ND	2.22	127.12	124.37
3	A	202	HEM	C3B-C4B-NB	-2.22	107.88	109.47
4	K	201	VXV	C05-C22-C02	-2.22	106.21	108.18
3	E	201	HEM	C3B-C4B-NB	-2.21	107.88	109.47
4	D	203	VXV	O01-C02-N03	-2.21	119.29	125.60
3	F	201	HEM	C3D-C4D-ND	-2.20	107.76	110.17
4	J	201	VXV	C21-C22-C02	2.20	133.58	129.32
3	E	201	HEM	C3D-C4D-ND	-2.20	107.76	110.17
3	C	201	HEM	C4C-C3C-C2C	2.19	108.72	106.81
4	C	203	VXV	O23-C04-N03	-2.16	119.42	125.60
3	E	201	HEM	CHD-C4C-NC	2.16	126.81	124.45
3	L	201	HEM	C3B-C4B-NB	-2.14	107.93	109.47
3	A	202	HEM	C2D-C1D-ND	-2.14	107.44	109.90
4	K	201	VXV	C15-C13-CL14	-2.11	116.53	119.17
4	E	202	VXV	C05-C04-N03	2.11	113.01	105.32
4	A	203	VXV	C19-C06-N07	-2.10	118.71	121.33
4	B	202	VXV	O23-C04-N03	-2.10	119.59	125.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	201	HEM	C3D-C4D-ND	-2.10	107.87	110.17
3	D	202	HEM	C3B-C2B-C1B	2.10	107.98	106.41
3	F	201	HEM	CHD-C4C-NC	2.08	126.71	124.45
4	H	202	VXV	C08-N07-C06	2.07	128.38	123.35
3	C	201	HEM	CHA-C4D-ND	2.07	126.93	124.37
4	L	202	VXV	O23-C04-N03	-2.06	119.70	125.60
4	C	203	VXV	C05-C04-N03	2.05	112.80	105.32
3	A	202	HEM	CBB-CAB-C3B	-2.04	117.32	127.53
3	E	201	HEM	C2A-C1A-NA	-2.04	107.89	110.15
4	L	202	VXV	O01-C02-N03	-2.03	119.79	125.60
4	K	201	VXV	C13-C12-C11	-2.02	117.65	119.71
4	J	201	VXV	C08-N07-C06	2.01	128.23	123.35
4	C	202	VXV	C05-C04-N03	2.01	112.67	105.32
3	D	202	HEM	CAA-CBA-CGA	-2.01	108.33	113.67

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	203	VXV	N07-C08-C09-C10
4	C	203	VXV	C08-C09-C10-C11
4	K	201	VXV	C08-C09-C10-C11
4	F	202	VXV	N07-C08-C09-C10
3	D	202	HEM	CAA-CBA-CGA-O2A
3	D	202	HEM	CAA-CBA-CGA-O1A
3	H	201	HEM	CAA-CBA-CGA-O2A
3	A	202	HEM	CAA-CBA-CGA-O1A
3	D	202	HEM	CAD-CBD-CGD-O2D
3	H	201	HEM	CAA-CBA-CGA-O1A
3	C	201	HEM	CAA-CBA-CGA-O2A
3	A	202	HEM	CAD-CBD-CGD-O2D
3	D	202	HEM	CAD-CBD-CGD-O1D
3	C	201	HEM	CAA-CBA-CGA-O1A
3	L	201	HEM	CAD-CBD-CGD-O1D
3	A	202	HEM	CAD-CBD-CGD-O1D
3	L	201	HEM	CAD-CBD-CGD-O2D
3	E	201	HEM	CAA-CBA-CGA-O2A
3	E	201	HEM	CAD-CBD-CGD-O1D
3	E	201	HEM	CAD-CBD-CGD-O2D
3	F	201	HEM	CAD-CBD-CGD-O2D
3	F	201	HEM	CAD-CBD-CGD-O1D
3	A	202	HEM	CAA-CBA-CGA-O2A

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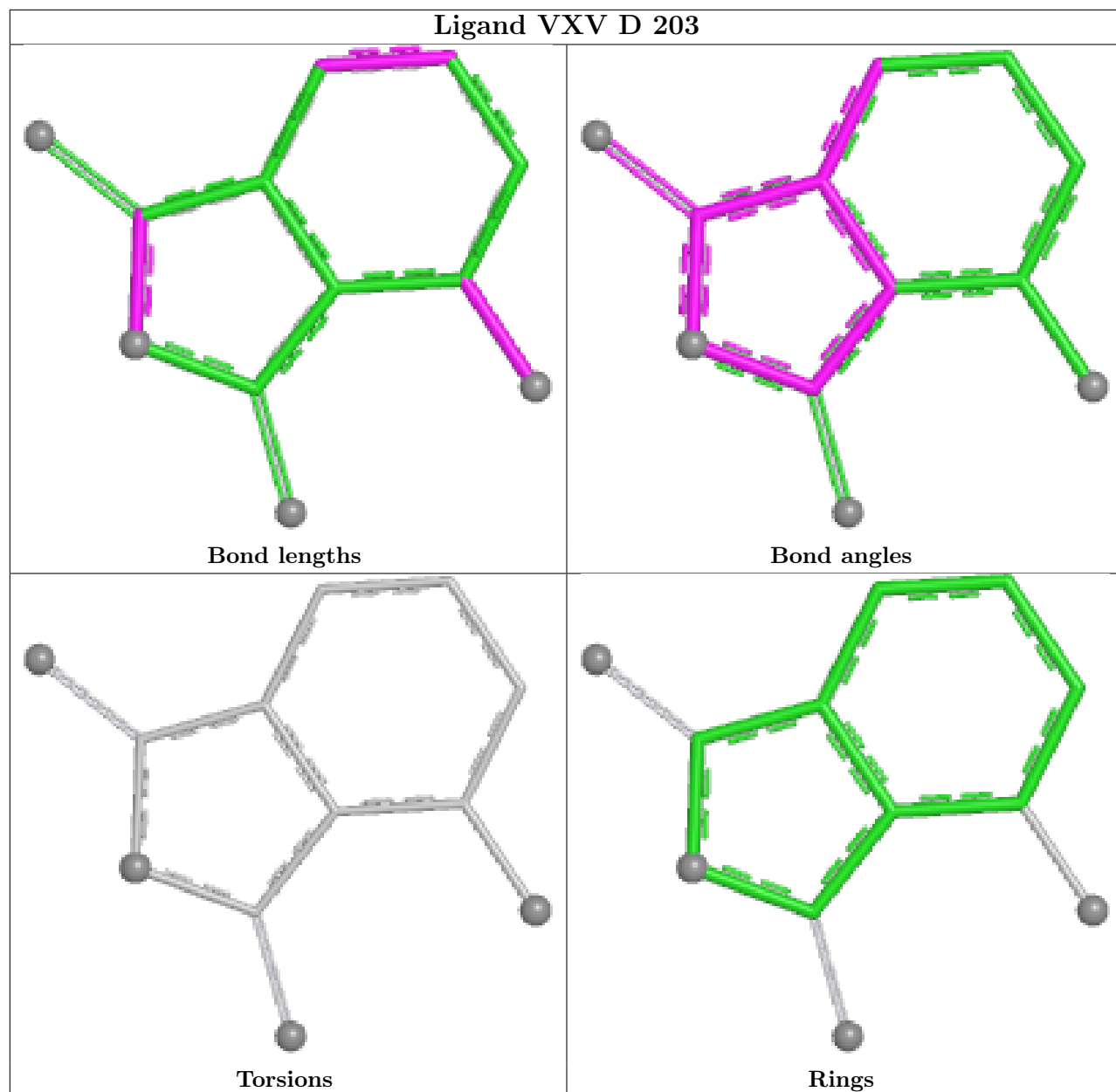
Mol	Chain	Res	Type	Atoms
3	H	201	HEM	CAD-CBD-CGD-O1D
3	F	201	HEM	CAA-CBA-CGA-O2A
3	H	201	HEM	CAD-CBD-CGD-O2D
3	F	201	HEM	CAA-CBA-CGA-O1A
3	E	201	HEM	CAA-CBA-CGA-O1A
3	L	201	HEM	CAA-CBA-CGA-O1A
3	L	201	HEM	CAA-CBA-CGA-O2A

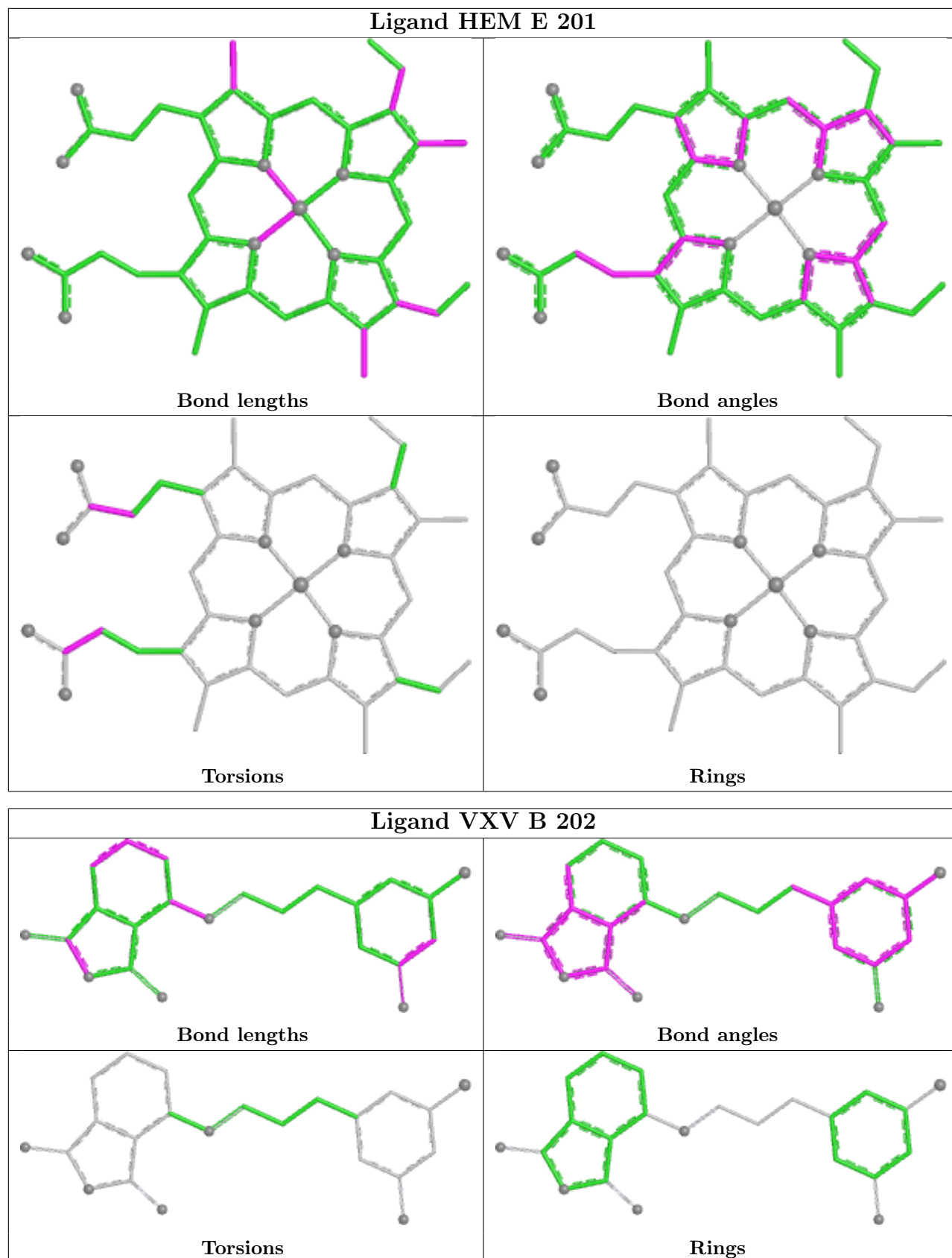
There are no ring outliers.

16 monomers are involved in 33 short contacts:

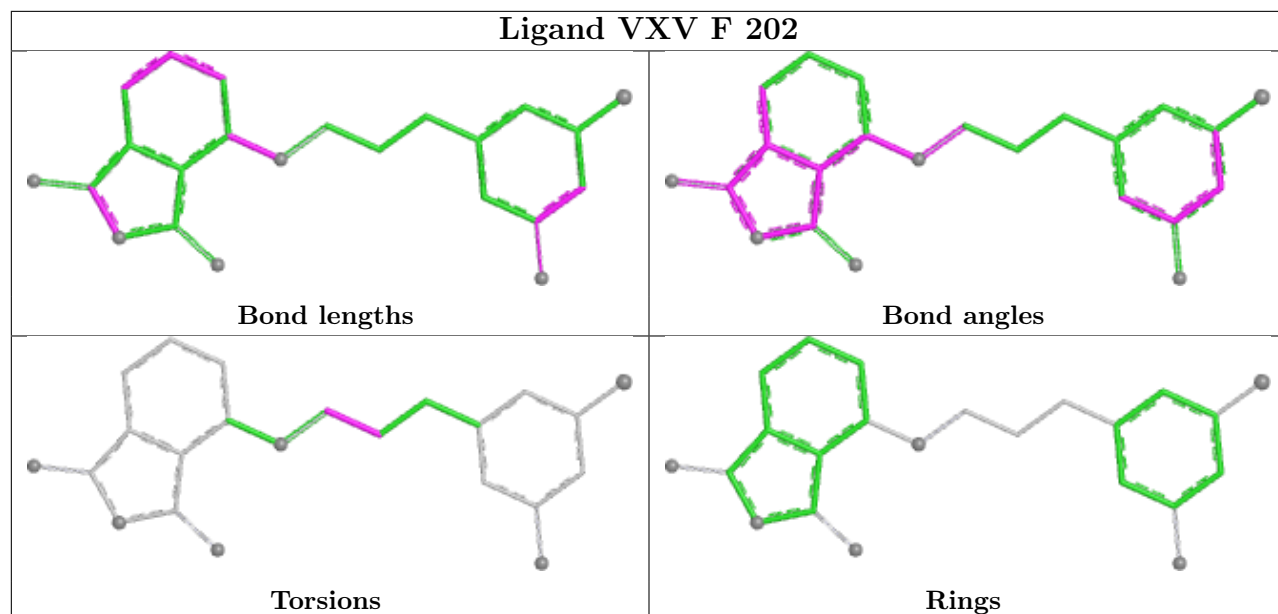
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	203	VXV	1	0
3	E	201	HEM	5	0
4	B	202	VXV	2	0
4	F	202	VXV	1	0
4	H	202	VXV	1	0
4	J	201	VXV	1	0
4	K	201	VXV	1	0
3	A	202	HEM	2	0
3	L	201	HEM	1	0
4	A	203	VXV	1	0
3	F	201	HEM	4	0
4	C	202	VXV	1	0
4	C	203	VXV	1	0
4	L	202	VXV	1	0
3	C	201	HEM	4	0
3	H	201	HEM	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

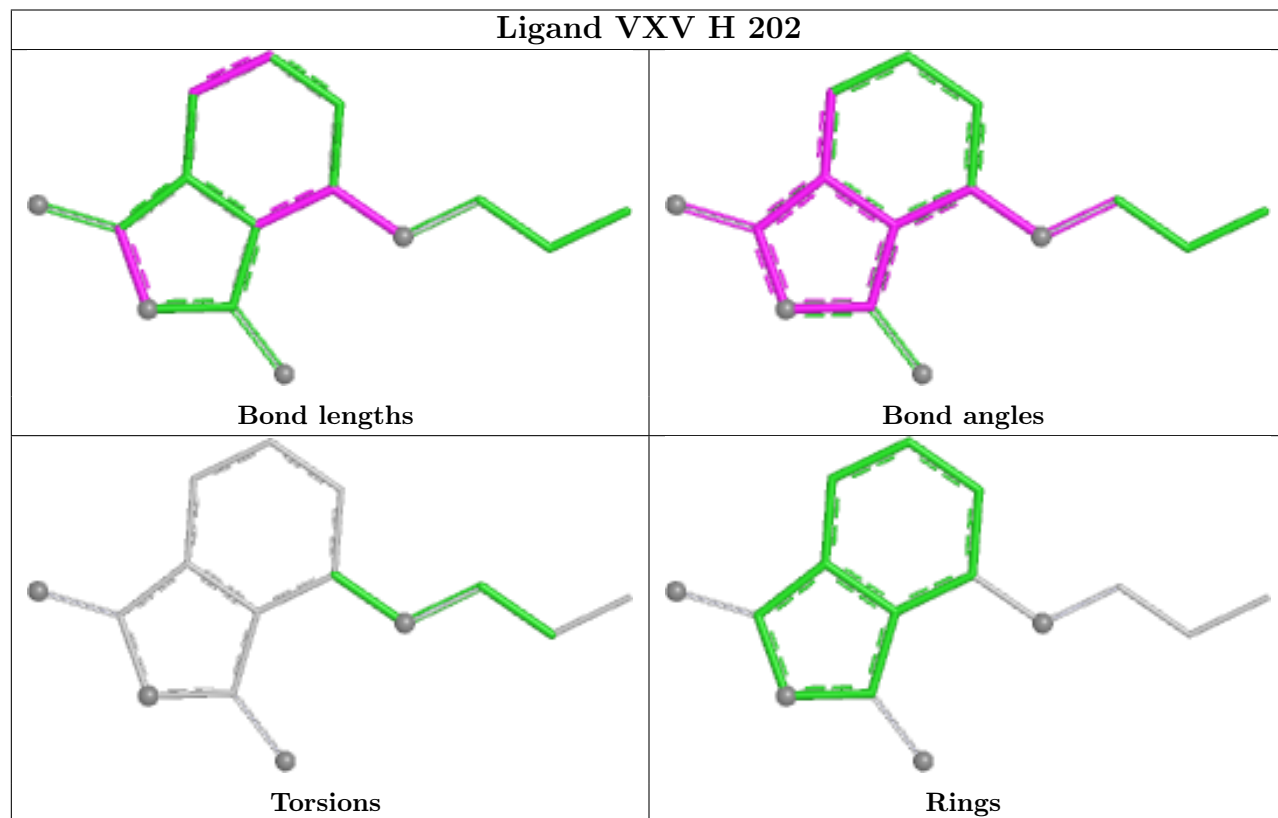




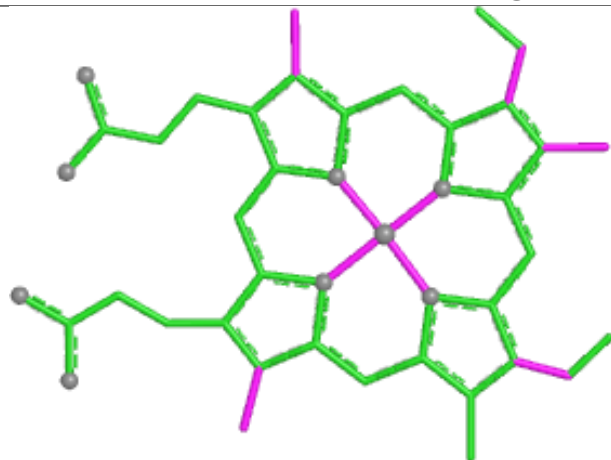
Ligand VXV F 202



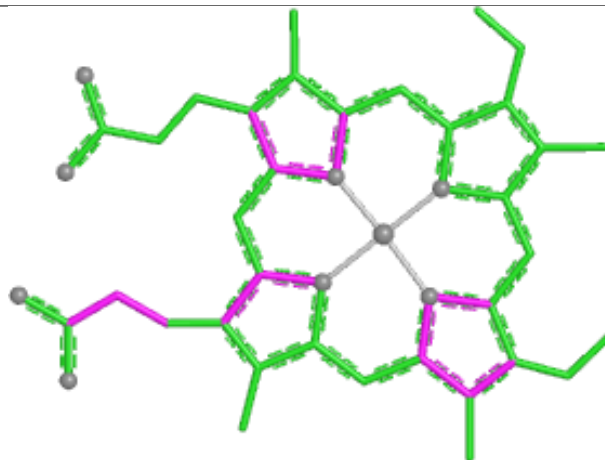
Ligand VXV H 202



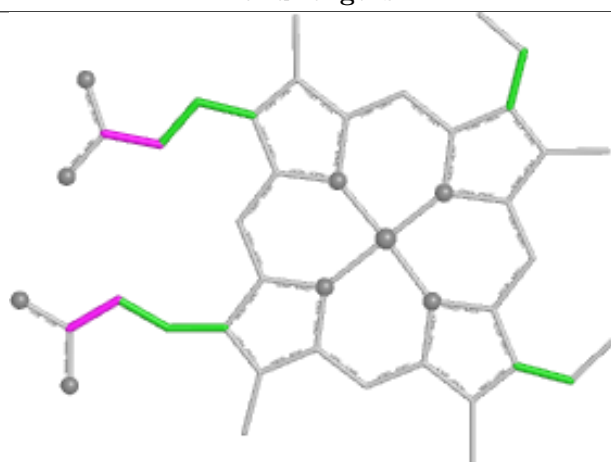
Ligand HEM D 202



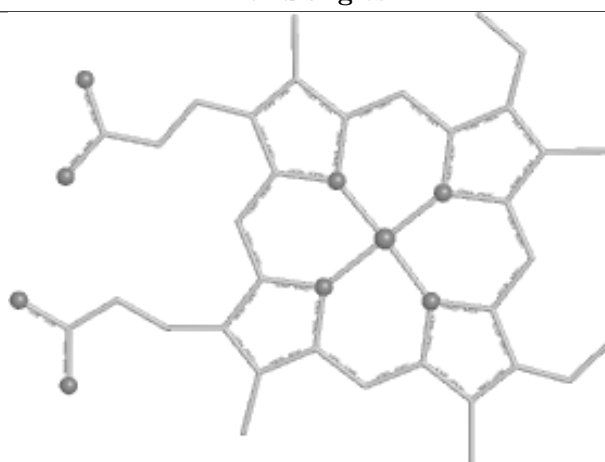
Bond lengths



Bond angles

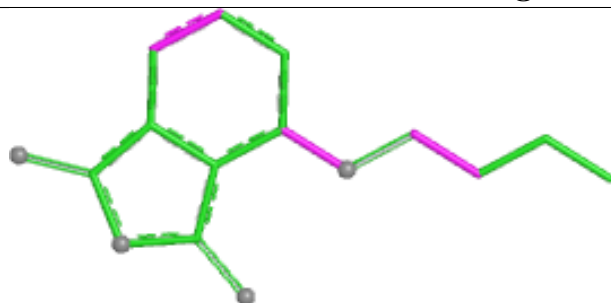


Torsions

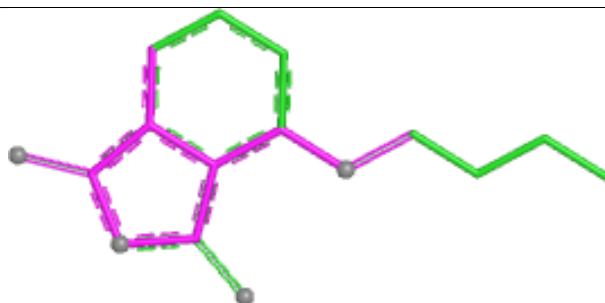


Rings

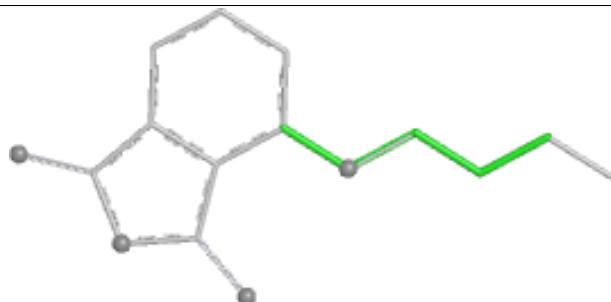
Ligand VXV J 201



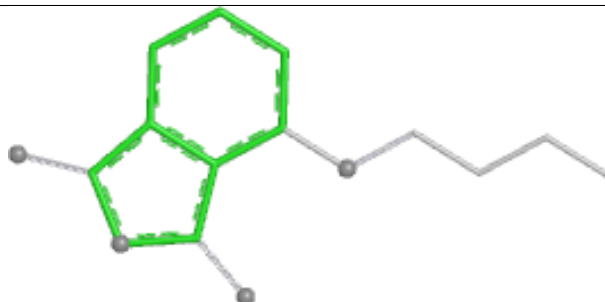
Bond lengths



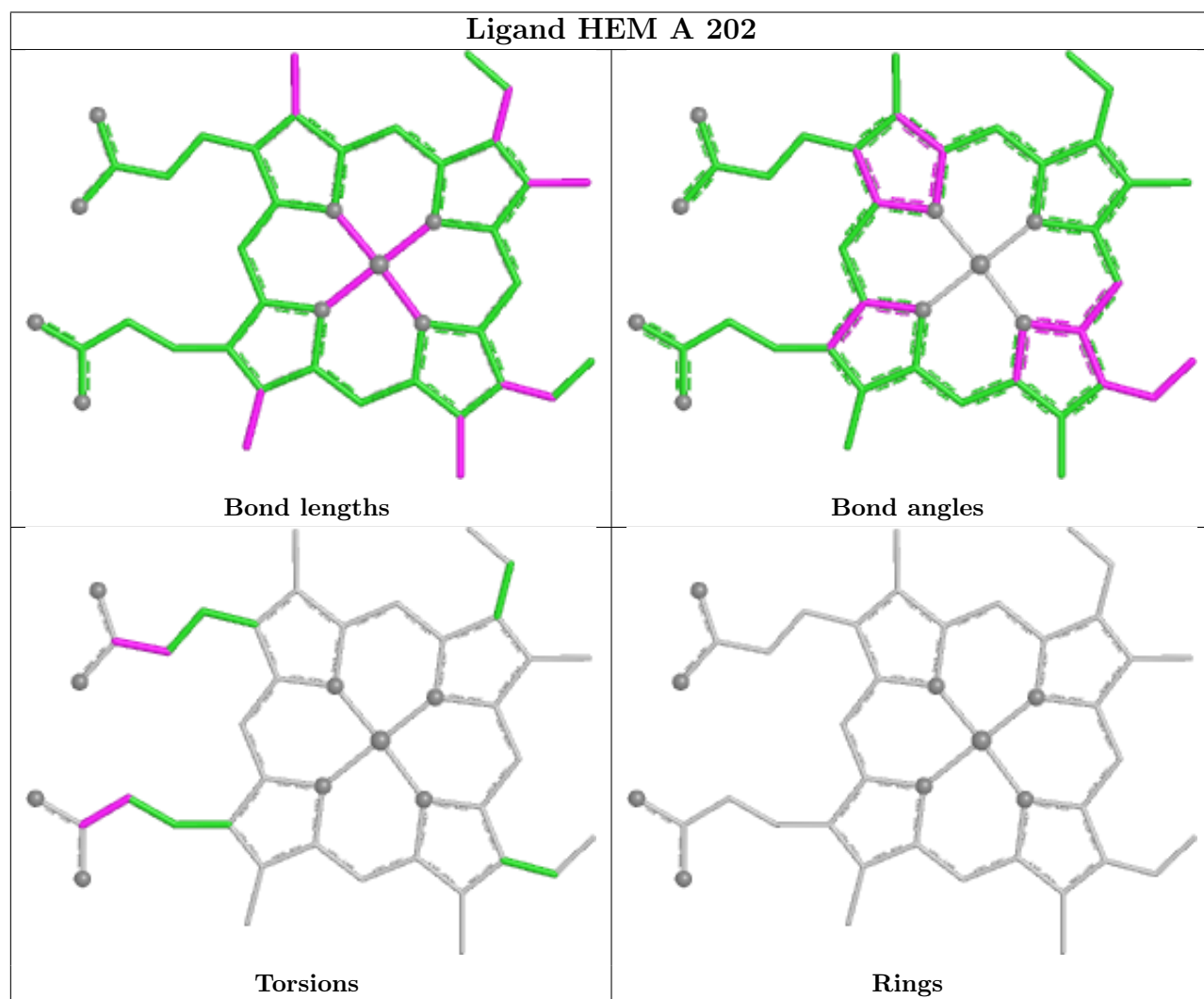
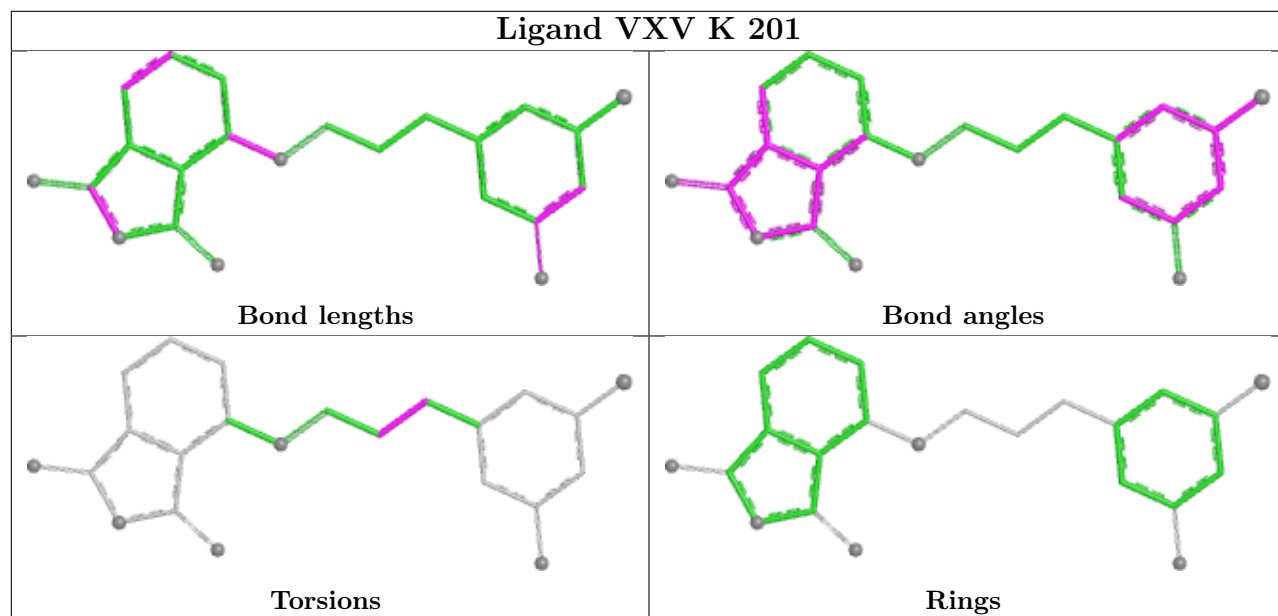
Bond angles

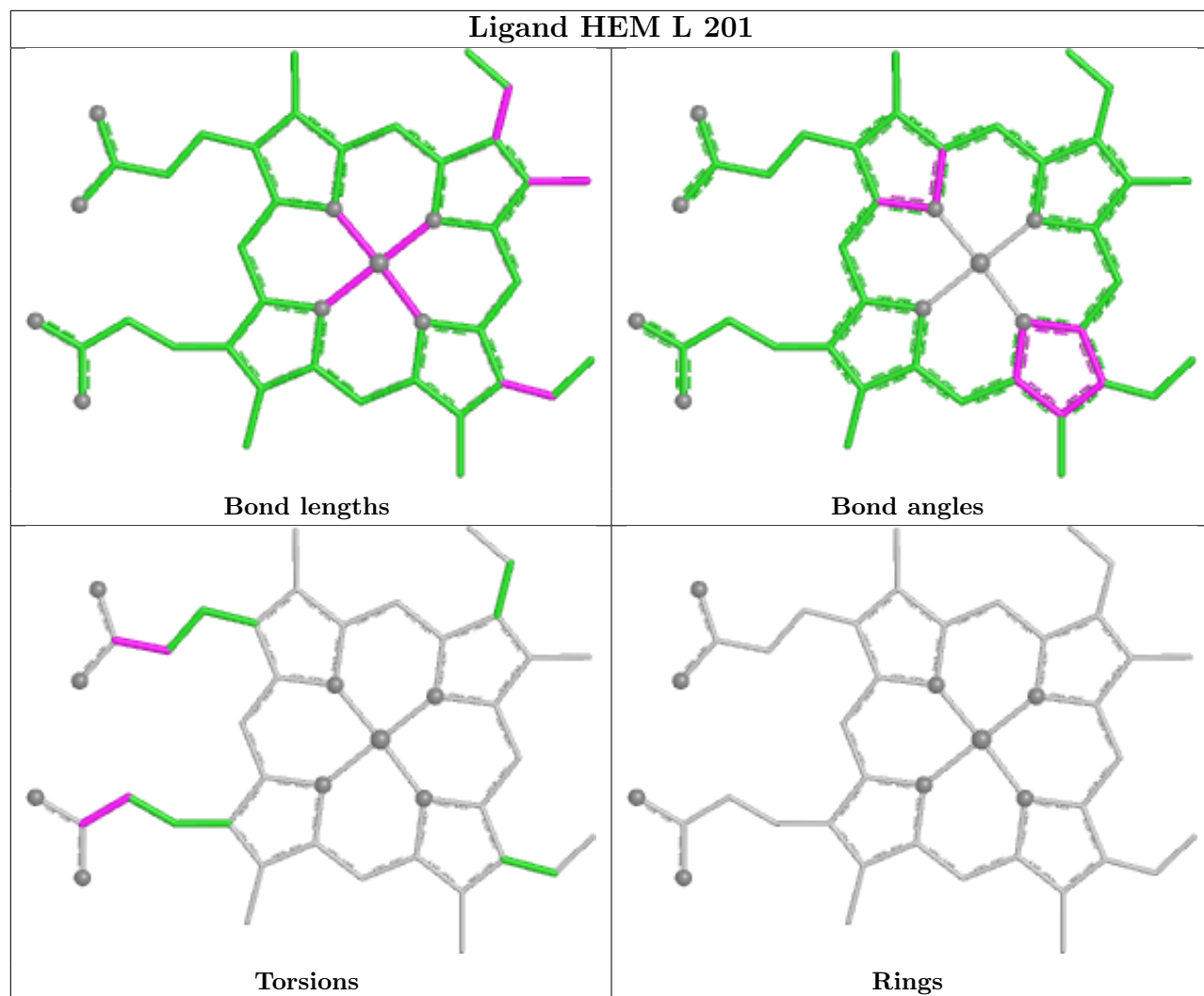


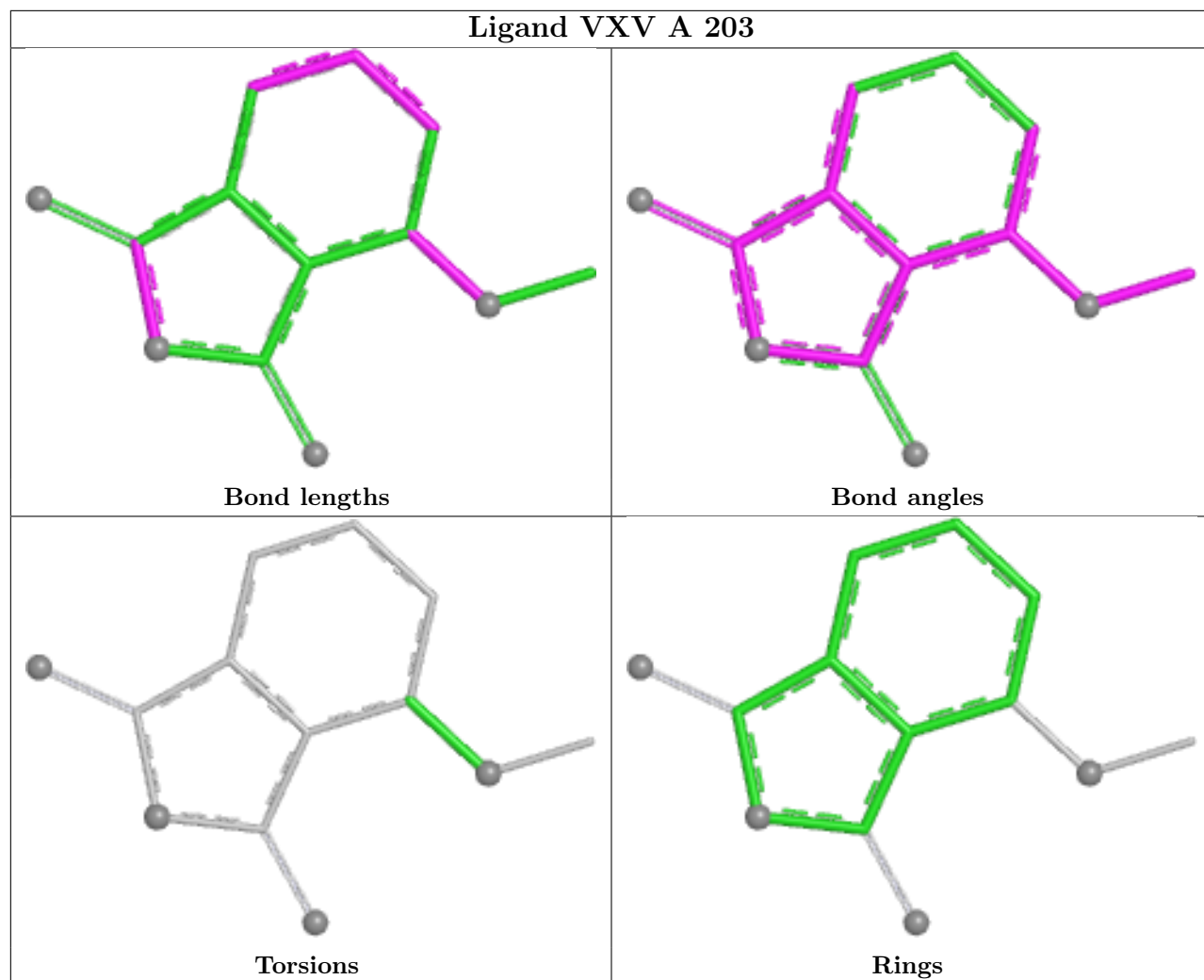
Torsions

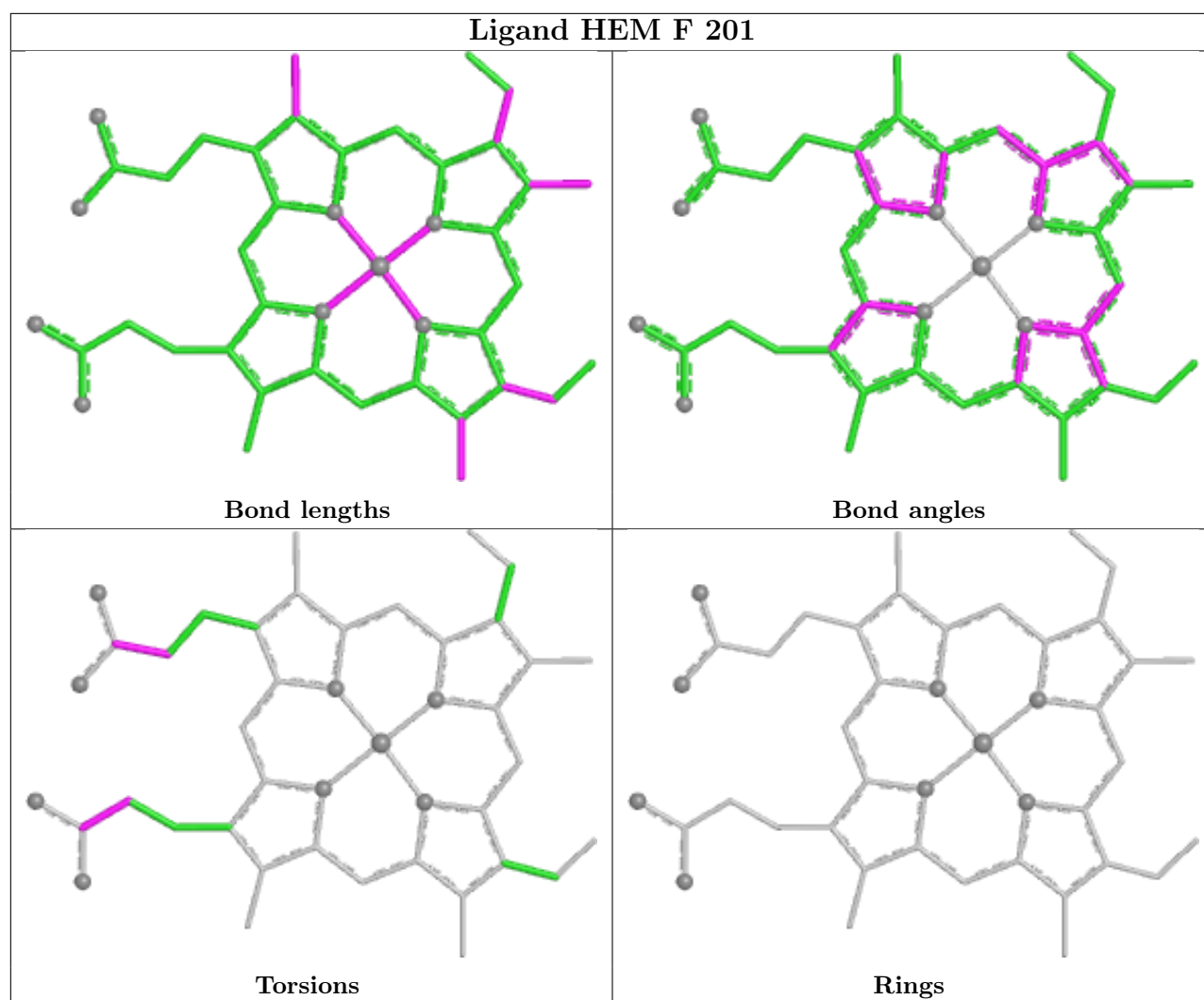


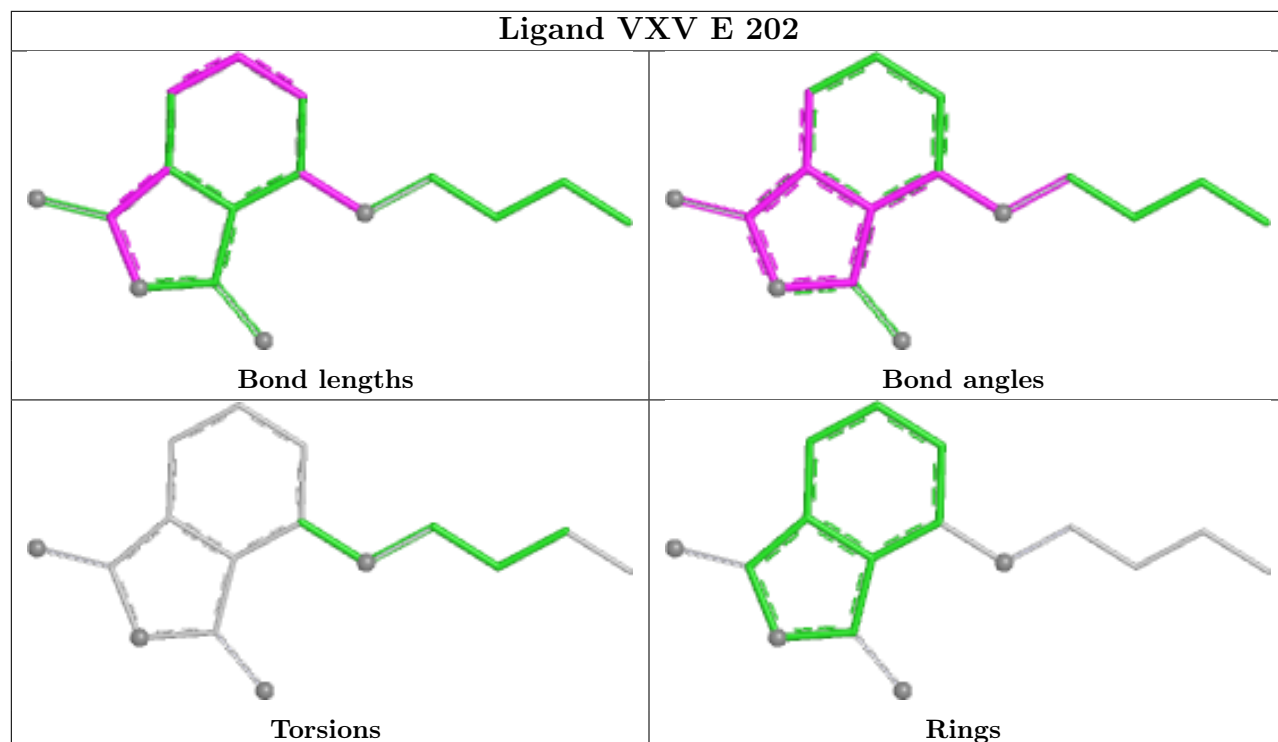
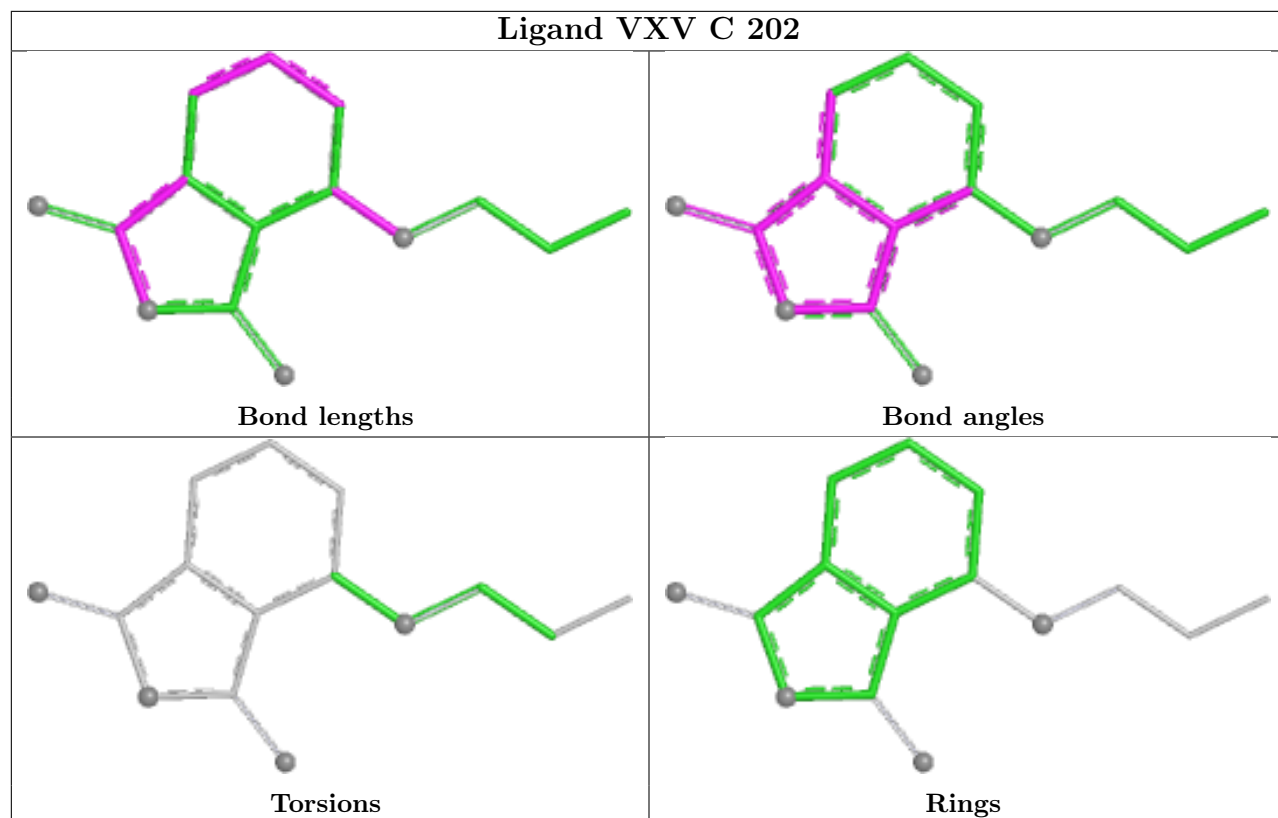
Rings

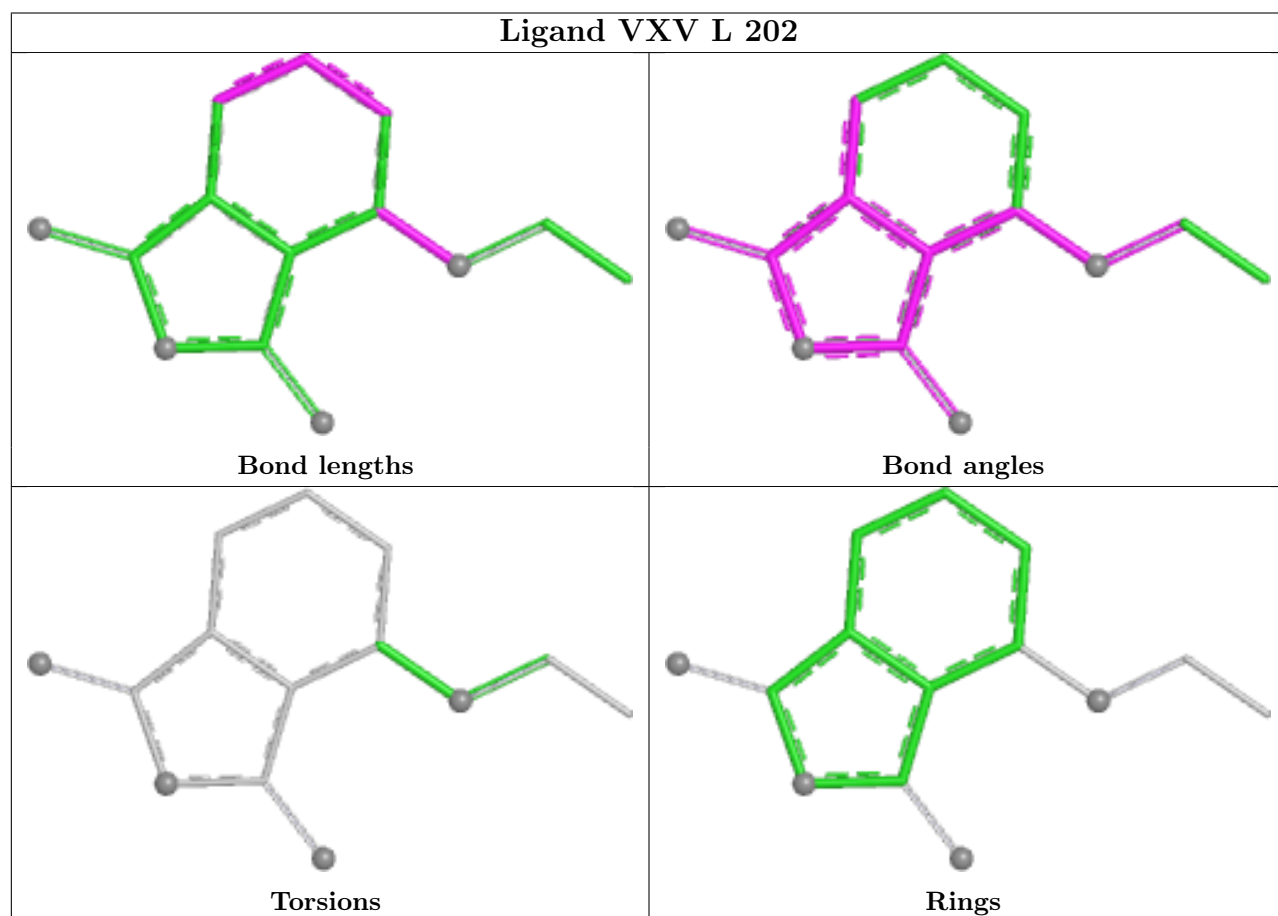
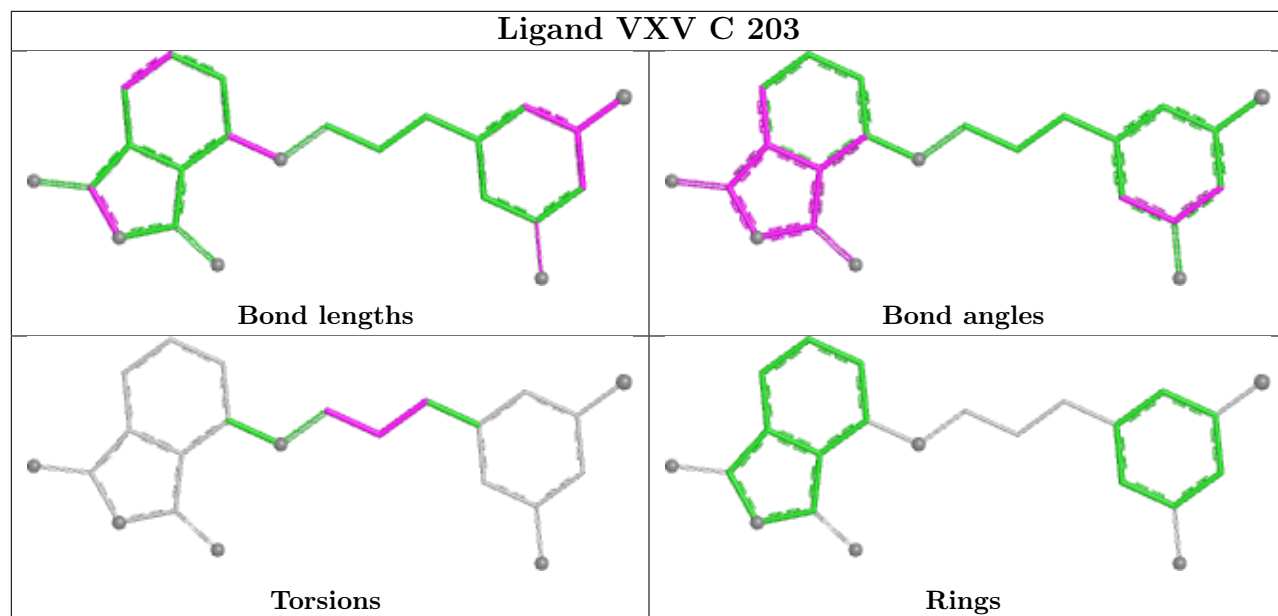


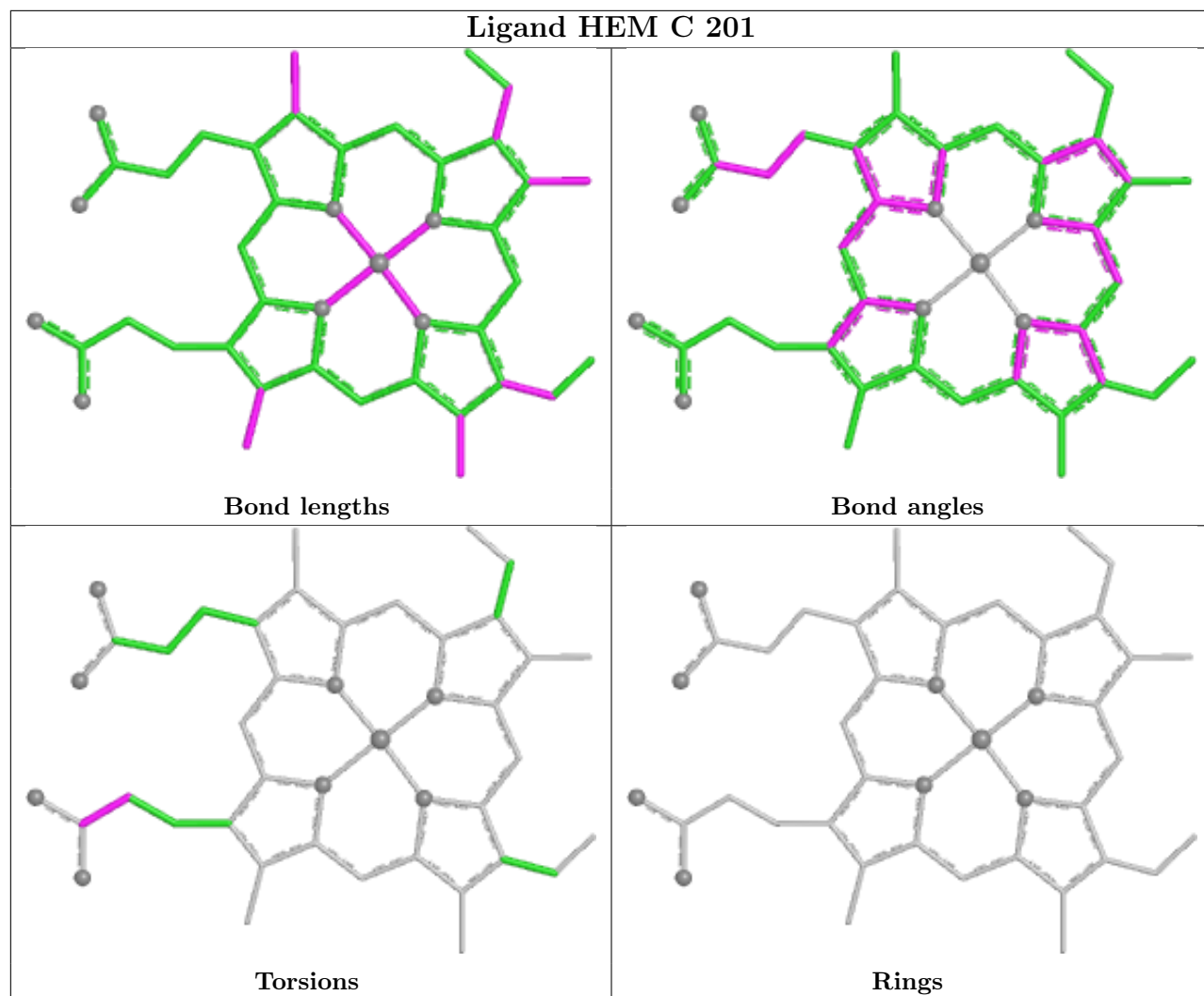


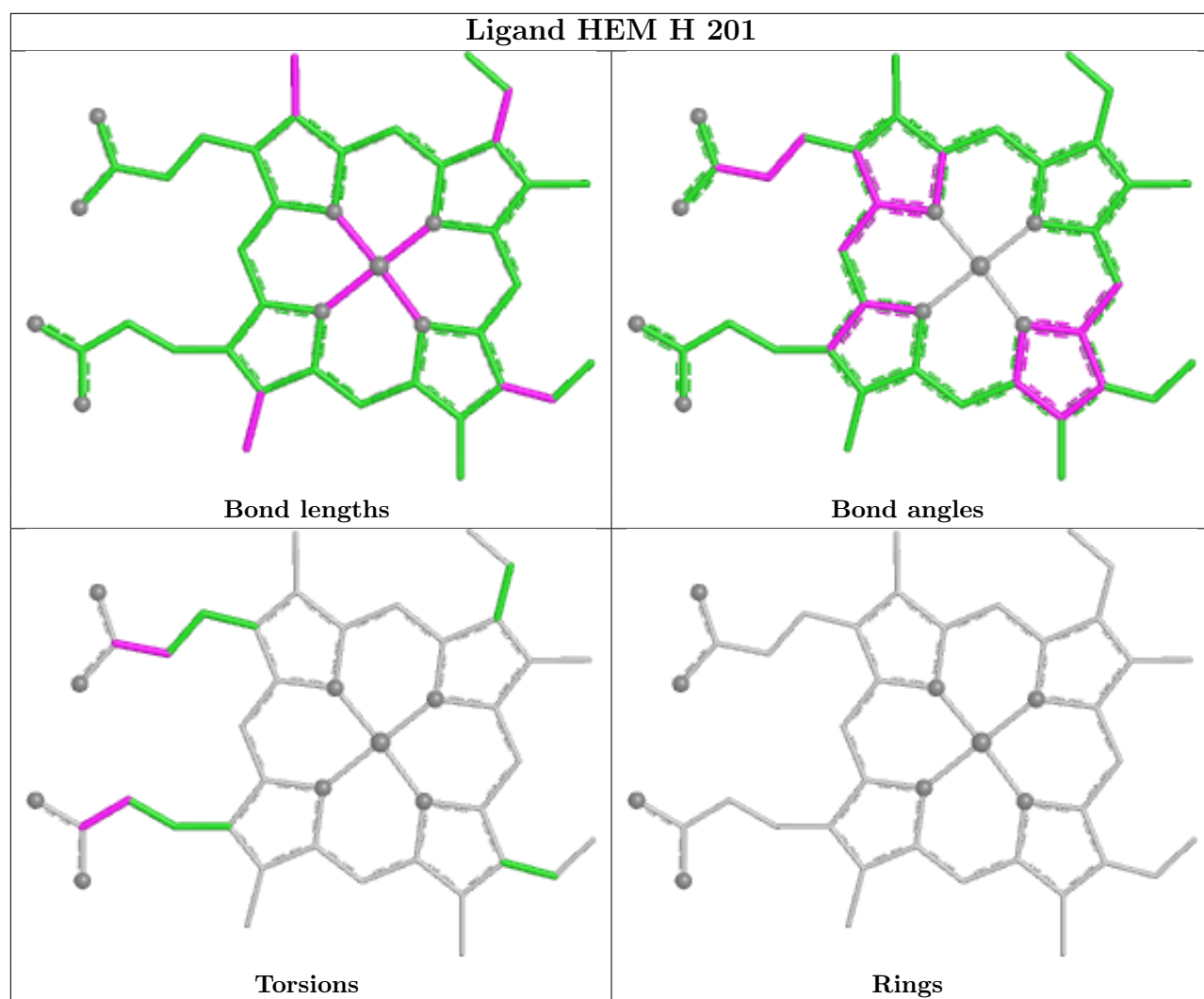












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	156/158 (98%)	-0.23	2 (1%) 75 78	16, 25, 36, 55	1 (0%)
1	B	156/158 (98%)	-0.24	2 (1%) 75 78	16, 25, 38, 55	1 (0%)
1	C	156/158 (98%)	-0.21	3 (1%) 66 70	14, 25, 36, 56	1 (0%)
1	D	156/158 (98%)	-0.11	1 (0%) 85 87	16, 27, 38, 59	1 (0%)
1	E	156/158 (98%)	-0.31	1 (0%) 85 87	14, 23, 34, 56	2 (1%)
1	F	156/158 (98%)	-0.25	1 (0%) 85 87	15, 26, 36, 58	1 (0%)
1	G	156/158 (98%)	-0.23	2 (1%) 75 78	15, 25, 36, 58	1 (0%)
1	H	156/158 (98%)	-0.21	1 (0%) 85 87	14, 26, 37, 58	2 (1%)
1	I	156/158 (98%)	-0.14	1 (0%) 85 87	15, 26, 37, 60	1 (0%)
1	J	156/158 (98%)	-0.24	1 (0%) 85 87	15, 25, 35, 58	1 (0%)
1	K	156/158 (98%)	-0.23	1 (0%) 85 87	16, 26, 35, 61	1 (0%)
1	L	156/158 (98%)	-0.18	3 (1%) 66 70	14, 25, 35, 61	2 (1%)
All	All	1872/1896 (98%)	-0.21	19 (1%) 79 82	14, 25, 36, 61	15 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	156	GLU	3.2
1	L	80	GLY	3.0
1	C	156	GLU	3.0
1	E	156	GLU	2.9
1	L	155	HIS	2.8
1	G	156	GLU	2.6
1	A	156	GLU	2.4
1	K	156	GLU	2.4
1	A	155	HIS	2.4
1	B	80	GLY	2.4
1	H	156	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	79	ILE	2.2
1	D	155	HIS	2.2
1	F	156	GLU	2.1
1	C	155	HIS	2.1
1	B	156	GLU	2.1
1	J	156	GLU	2.1
1	G	155	HIS	2.0
1	I	80	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

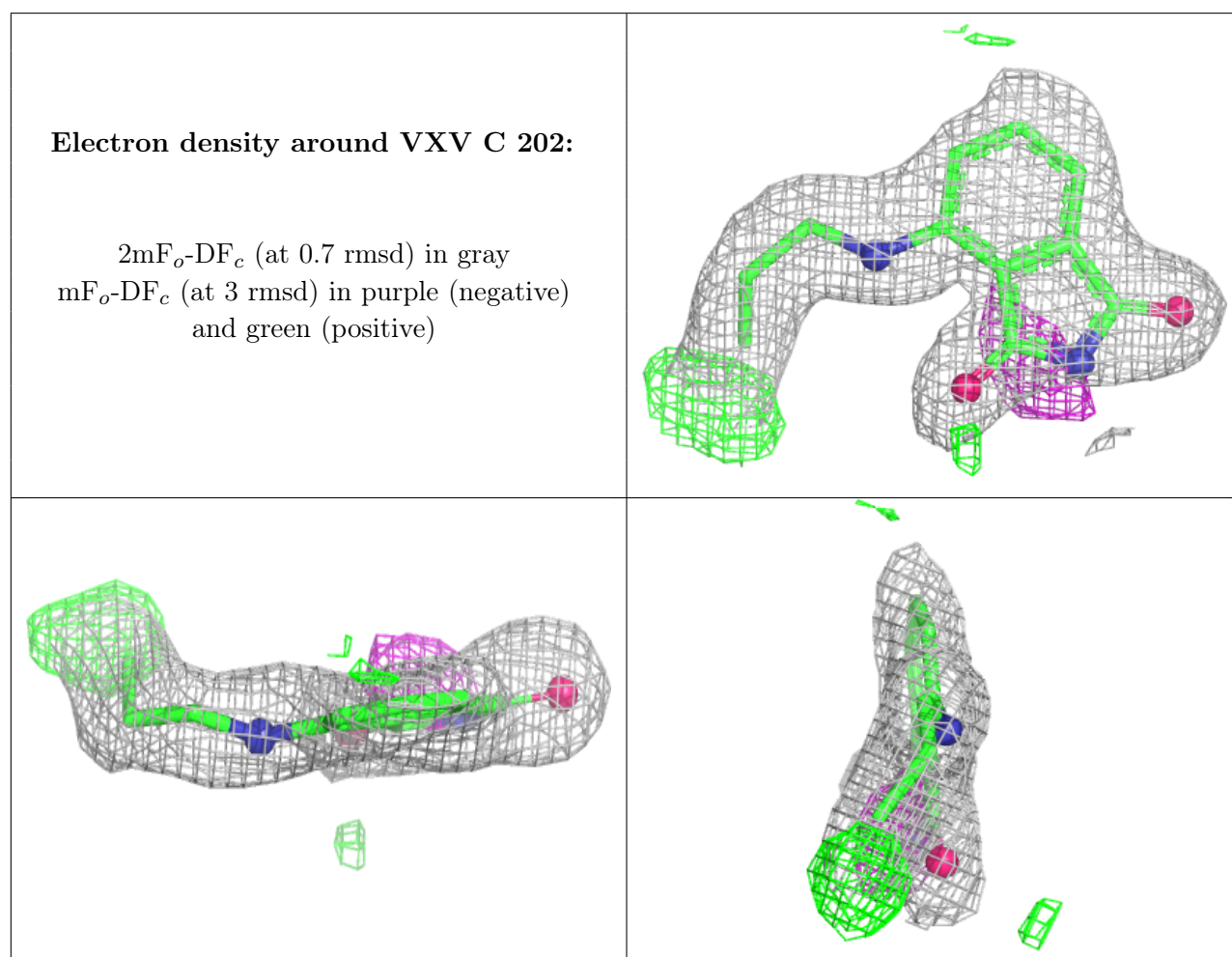
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	VXV	C	202	15/23	0.75	0.19	29,46,51,52	0
4	VXV	E	202	16/23	0.77	0.17	33,46,54,63	0
4	VXV	A	203	13/23	0.79	0.15	29,41,51,52	0
4	VXV	H	202	15/23	0.79	0.16	34,44,52,52	0
4	VXV	F	202	23/23	0.81	0.16	33,48,70,95	0
4	VXV	C	203	23/23	0.83	0.15	33,47,64,71	0
4	VXV	B	202	23/23	0.84	0.15	29,48,68,94	0
4	VXV	J	201	16/23	0.85	0.14	36,47,54,54	0
4	VXV	K	201	23/23	0.85	0.15	37,51,77,88	0
4	VXV	L	202	14/23	0.86	0.13	29,40,47,53	0
4	VXV	D	203	12/23	0.90	0.11	37,43,50,51	0
3	HEM	L	201	43/43	0.95	0.11	24,28,39,46	43
3	HEM	A	202	43/43	0.95	0.10	24,28,50,56	0
3	HEM	C	201	43/43	0.95	0.10	25,28,46,64	0
3	HEM	D	202	43/43	0.95	0.10	28,34,50,53	43

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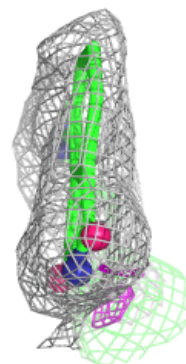
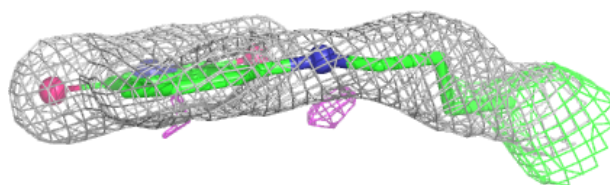
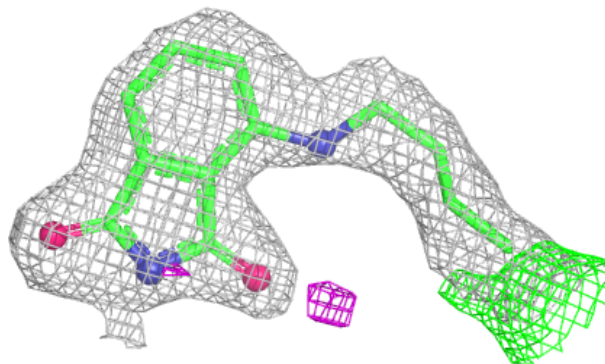
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	HEM	F	201	43/43	0.95	0.10	23,28,47,53	0
3	HEM	H	201	43/43	0.95	0.11	23,29,51,62	0
3	HEM	E	201	43/43	0.96	0.10	21,27,48,57	0
2	K	A	201	1/1	1.00	0.02	17,17,17,17	0
2	K	B	201	1/1	1.00	0.02	18,18,18,18	0
2	K	D	201	1/1	1.00	0.02	20,20,20,20	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



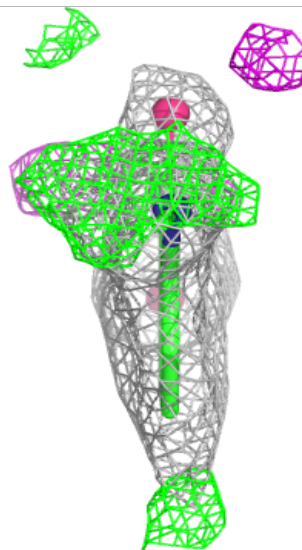
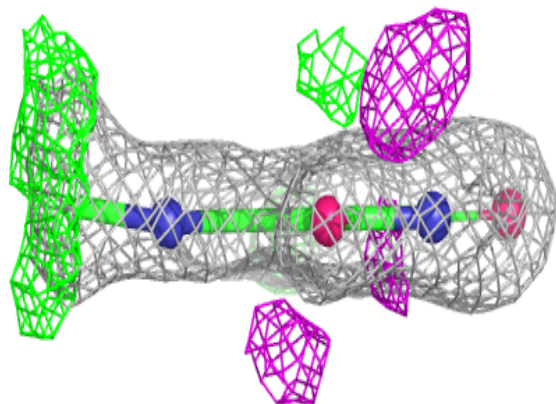
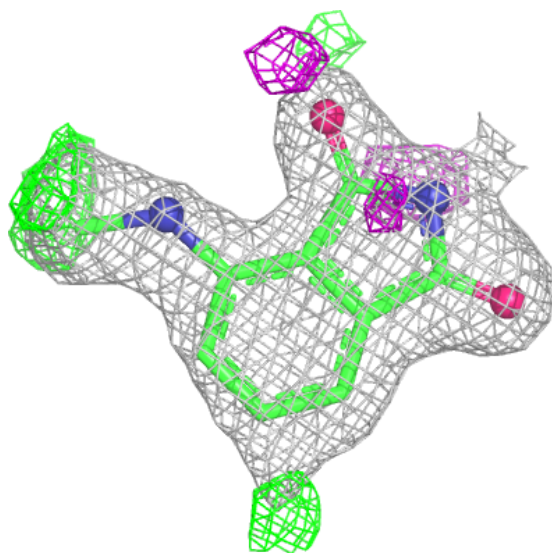
Electron density around VXV E 202:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



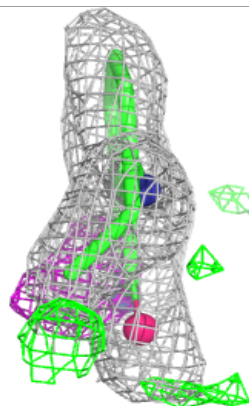
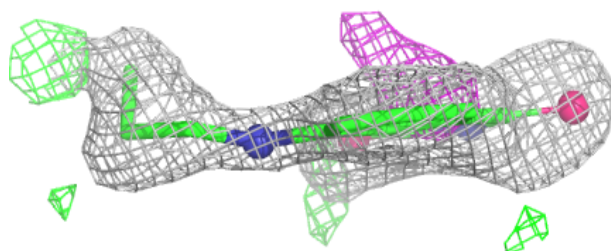
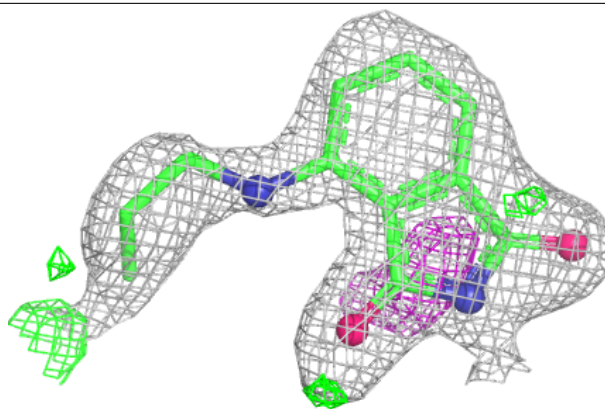
Electron density around VXV A 203:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

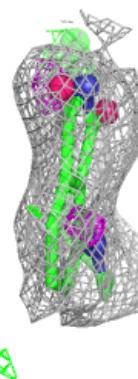
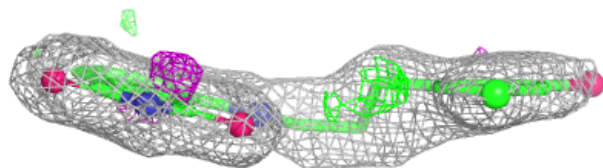
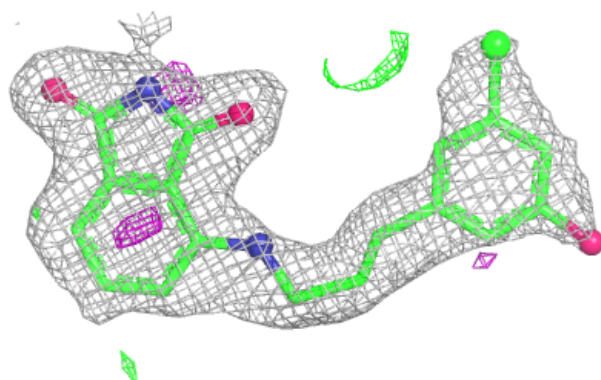


Electron density around VXV H 202:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

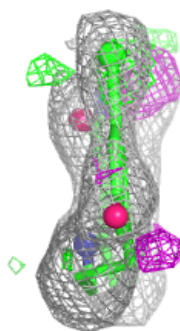
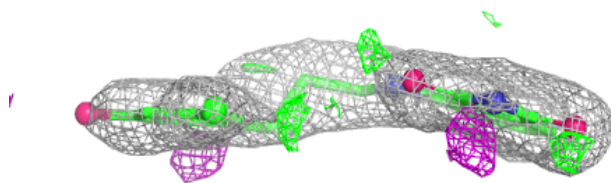
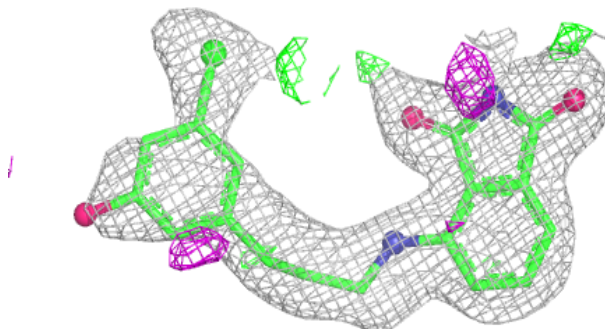
**Electron density around VXV F 202:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

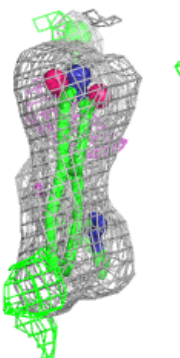
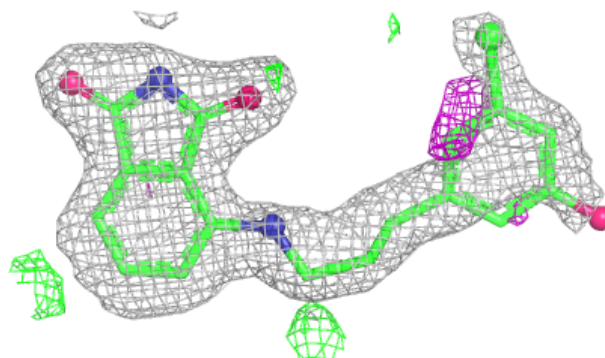


Electron density around VXV C 203:

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 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
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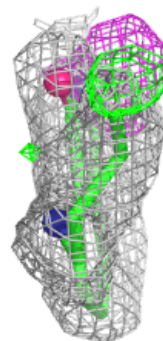
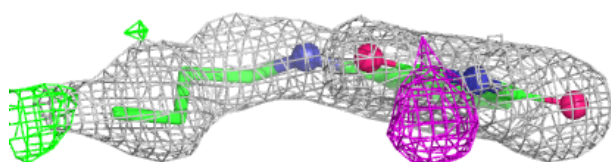
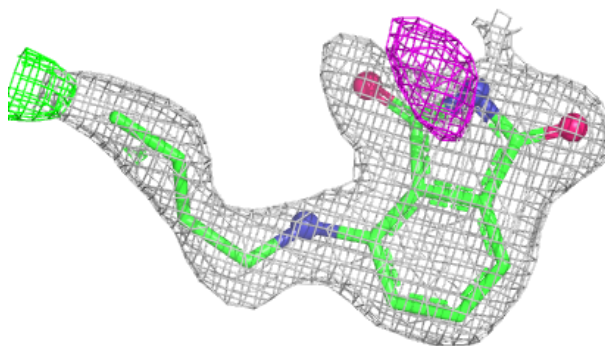
**Electron density around VXV B 202:**

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 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

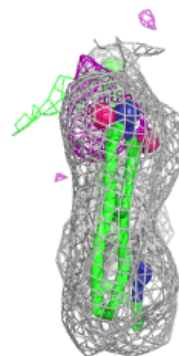
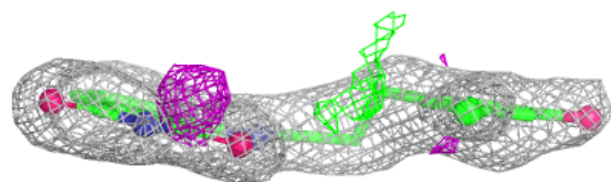
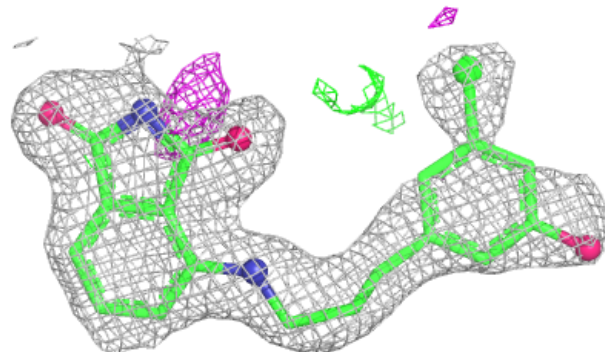


Electron density around VXV J 201:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

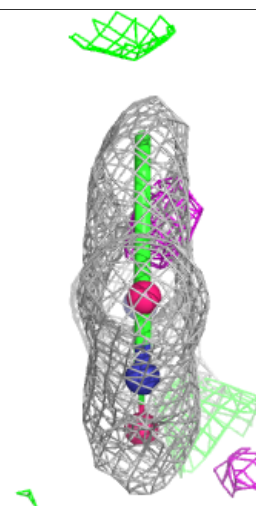
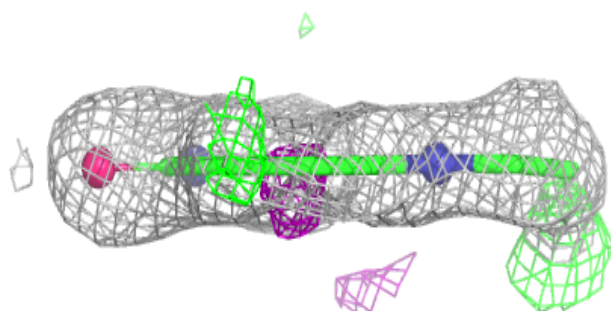
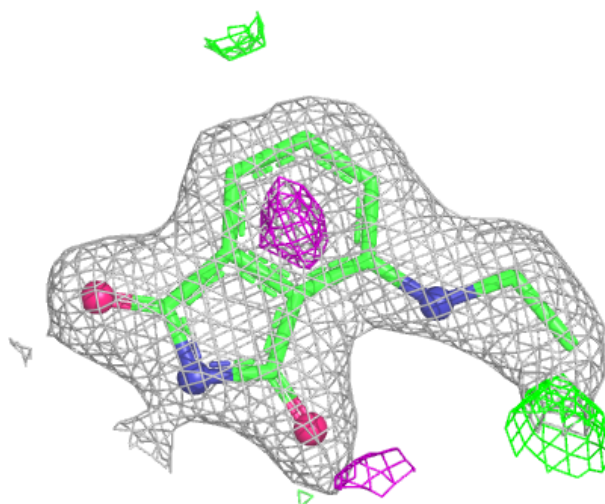
**Electron density around VXV K 201:**

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and green (positive)



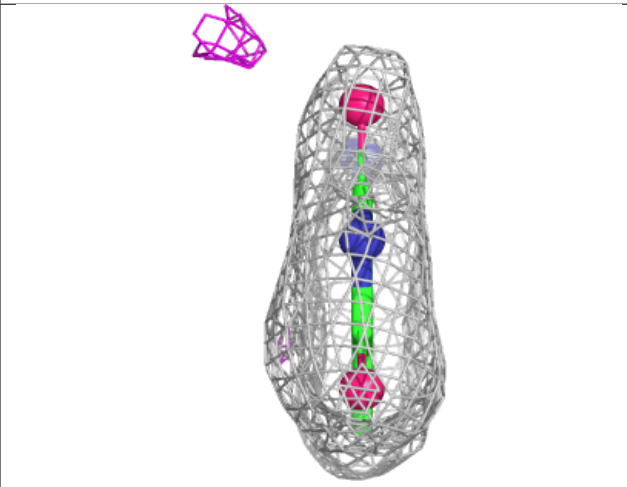
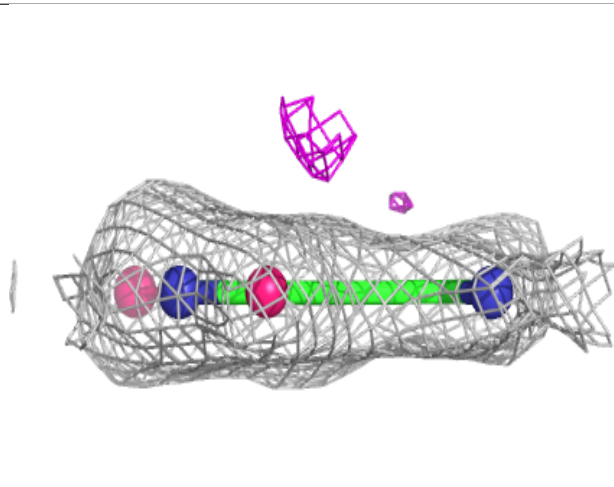
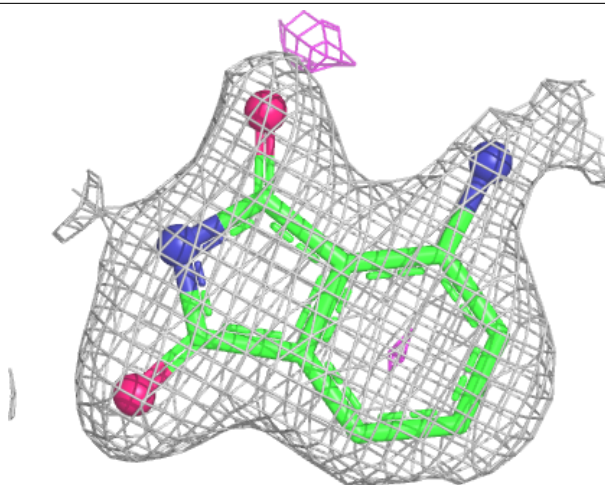
Electron density around VXV L 202:

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and green (positive)



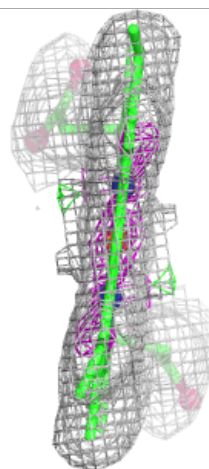
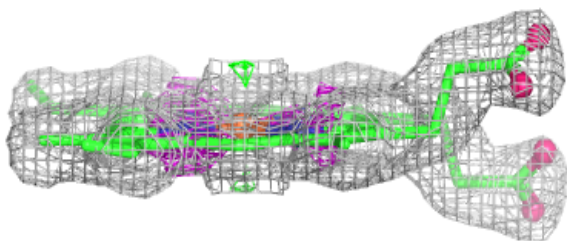
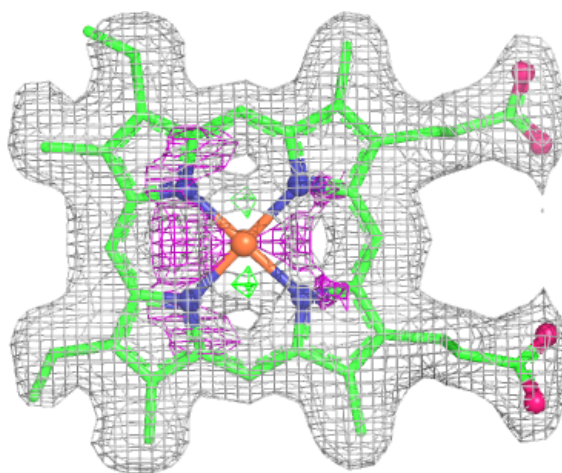
Electron density around VXV D 203:

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and green (positive)



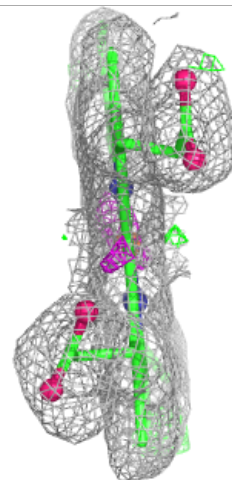
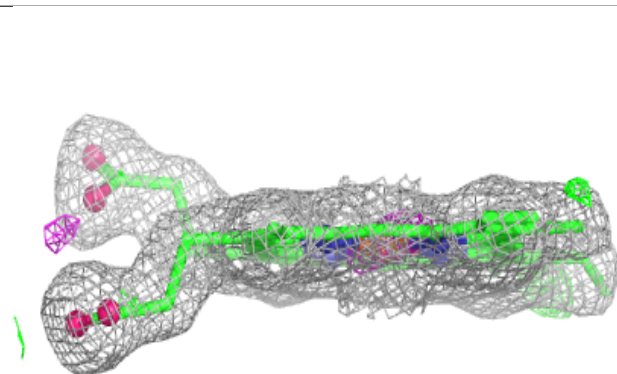
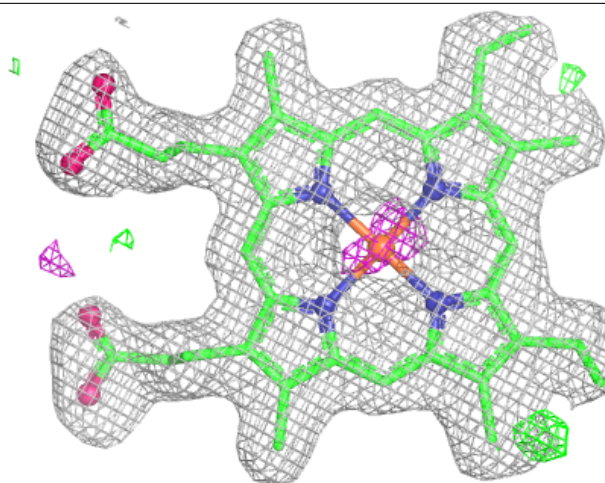
Electron density around HEM L 201:

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and green (positive)



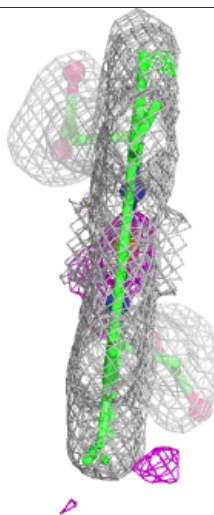
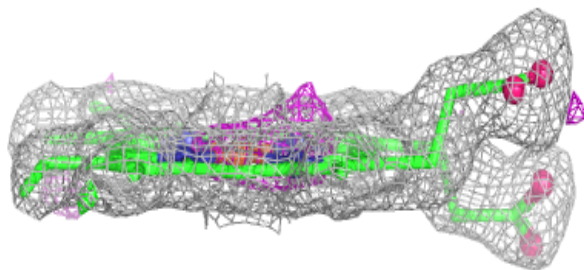
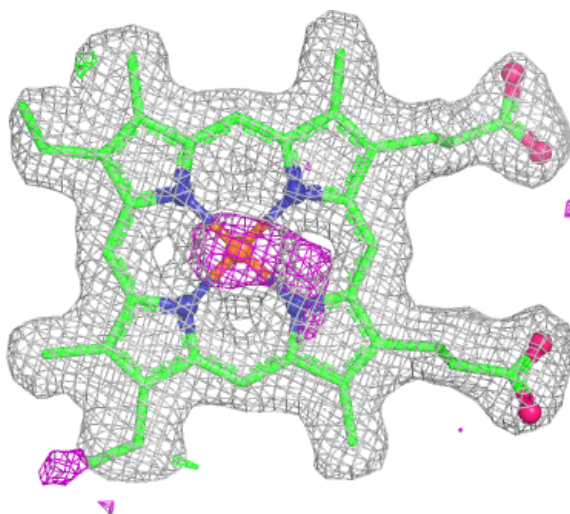
Electron density around HEM A 202:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



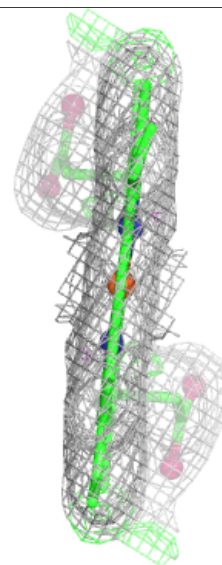
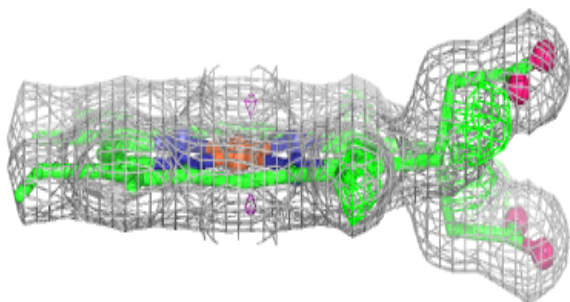
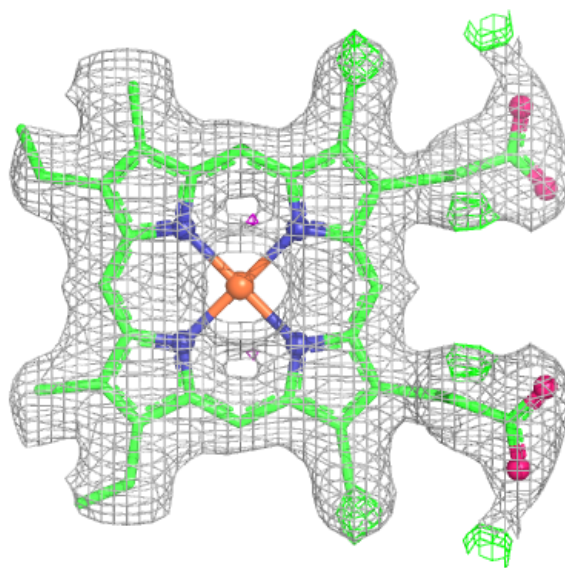
Electron density around HEM C 201:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



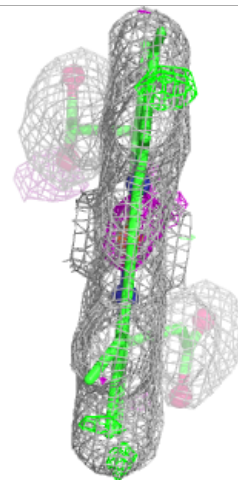
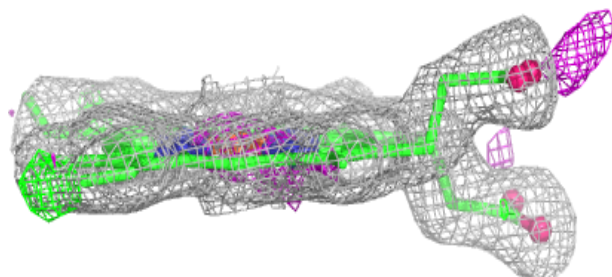
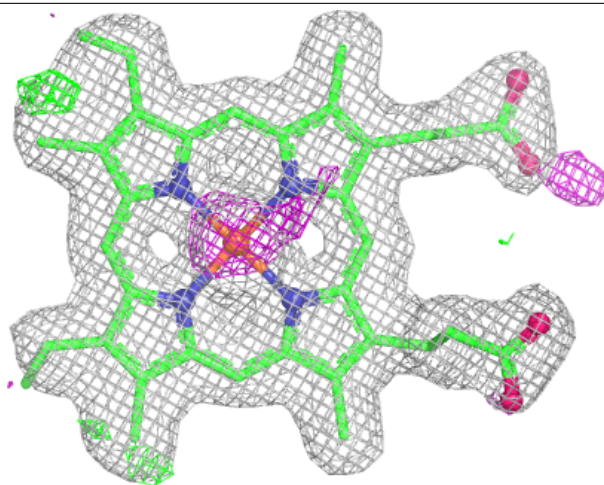
Electron density around HEM D 202:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



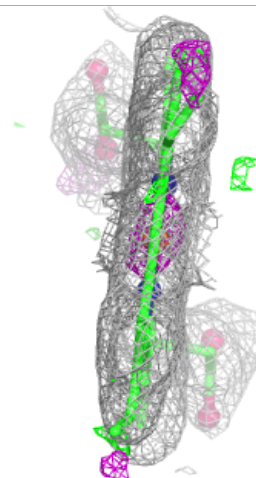
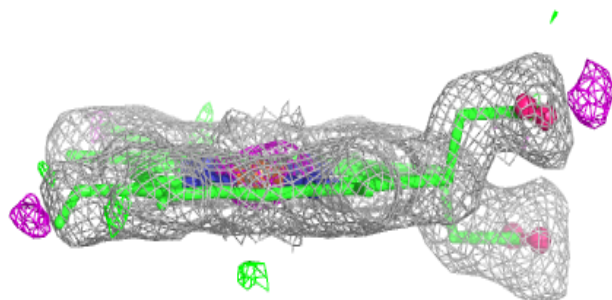
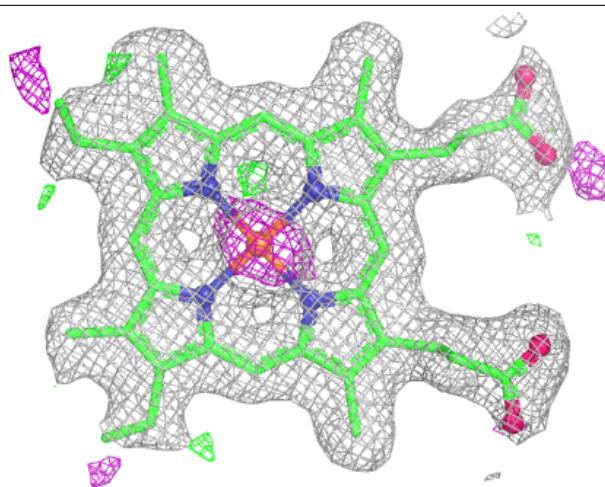
Electron density around HEM F 201:

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and green (positive)



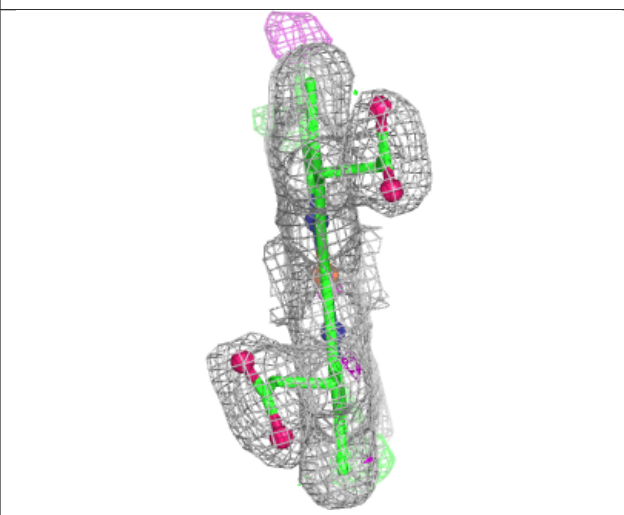
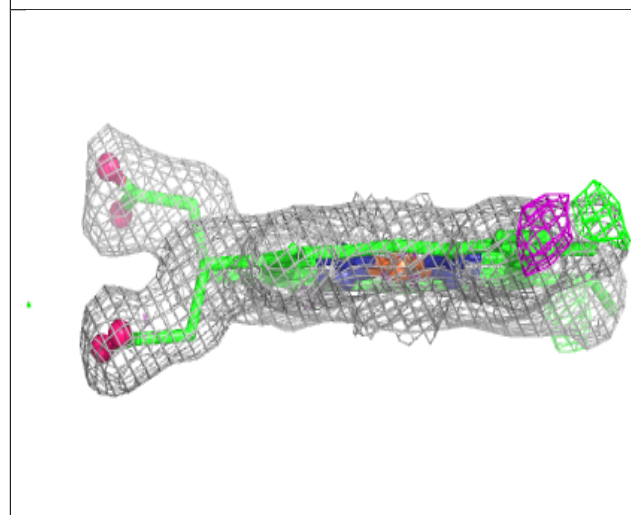
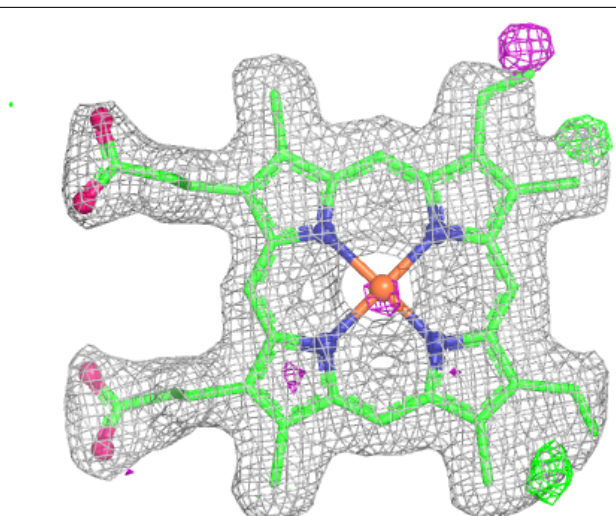
Electron density around HEM H 201:

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and green (positive)



Electron density around HEM E 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.